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Statistical Mechanics of Phase Transition

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Mayer's theory about the relation between the phase transitions and the singular points has been criticized. The matrix method is connected with Mayer's cluster theory applied to regular solutions. It is shown that the following two cases are possible. They are

i) that the density of atoms is a single analytic function of the active number density, at least, on the positive real axis, and the first singularity of this function is an essential singular point and the phase transition occurs at this point,

ii) that the density of atoms may consist of different analytic functions of the active number density, and the phase transition may occur at the point which is not analytic singular point of the function.

The same is true of continuous aggregate systems such as imperfect gases. In the continuous case the partition function may be obtained as the smallest eigenvalue of Fredholm's integral equation.

§ 1. Introduction

The existing theories, which deal with the systems composed of strongly interacting particles, such as imperfect gases, liquids and crystalline solids, are classified into three types, except very simple ones. The first of them is the integral equation method developed by Kirkwood[1], Yvon[2] and Born and Green[3]. This method is only approximative, and we can place trust in not all of quantitative results of it, since the Kirkwood approximation is utilized in this method. The same is true of the customary approximate theories applied to crystal statistics, such as Bethe's theory. The next is the matrix method elaborated by Krammers and Wannier[4], Montroll[5], Lassettre and Howe[6], Onsager[7] and others. This method is strict, but applicable only to the case of crystal statistics. The last one is the method of cluster intagrals of Mayer[8,9], which is considered as the most general one. This method is, however, not so useful for practical calculations and some of its important conclusions have been drawn without complete proof, as pointed out by Katsura and Fujita[10].

The purposes of the present paper are to criticize the results of Mayer's theory about the relation between the phase transitions and the singular points, to investigate properties of the singularities in detail, and to give the proper statistical interpretation of the phase transition. Since the matrix method seems to give more definitive conclusion, we may make clear the ambiguous points of Mayer's theory if we connect the matrix method with Mayer's method of series developments. Since the matrix method is established only for the case of crystal statistics, we shall, at first, study the connection between these two methods for this case. And an attempt to extend the eigenvalue method to continuous aggregate systems will be discussed in the last portion of this paper.

§ 2. Phase change and singularity

In this paper we shall consider a single-component system. If we denote by $\Xi(T, z, V)$ the grand partition function of it as a function of the absolute temperature T, the active number density* z, and the volume V, the pressure is written as

$$pV=kT\ln\Xi(T, z, V), \tag{1}$$

k being Boltzmann's constant. And if the classical laws of mechanics are applied to the system, the grand partition function $\Xi(T, z, V)$ is given by

$$\Xi(T, z, V)=\sum_{r=0}^{\infty}\frac{z^r}{r!}Q_r(T, V), \tag{2}$$

where $Q_r(T, V)$ is the configurational partition function of the system composed of the r molecules contained in the volume V. Here we assume that p is expressible as a power series in z as follows:

$$pV=kTV\sum_{s=1}^{\infty}b_s(T, V)z^s. \tag{3}$$

Then from the above relations, we see that the relation between $Q_r(T, V)$ and $V^s s!\, b_s(T, V)$ is the same as that between the r'th moment and the s'th Thiele semi-invariant in mathematical statistics[11]

$$Vb_s(T, V)=\sum[\textstyle\sum ir_i=s](-)^{\Sigma r_i-1}(\sum r_i-1)!\prod_{i=1}\left[\left(\frac{Q_i(T, V)}{i!}\right)^{r_i}\frac{1}{r_i!}\right], \tag{4}$$

where the sum extends over all sets of r_i such that $\sum ir_i=s$. If the potential energy is expressible as a sum of that between all pairs, $b_s(T, V)$ given by (4) agrees with Mayer's expression for the s'th cluster integral. This method is applicable also to the case of quantum statistics, and will give the result same as that Kahn and Uhlenbeck[12] have deduced.

If the volume is finite, and if two molecules cannot approach beyond a certain limit, a finite volume can contain only finite number of molecules. So $Q_r(T, V)$ vanishes for r larger than a certain value. And the $\Xi(T, z, V)$ is regular for all finite z of the complex plane, since it becomes polynomial in z. And (3) also is regular except at the zeros of (2).

If the intermolecular force is sufficiently short-ranged, $b_s(T, V)$ for every s is asymptotically independent of the volume. And it will approach a certain limiting value $b_s(T)$, if we let the volume be infinite:

$$b_s(T)=\lim_{V\to\infty}b_s(T, V). \tag{5}$$

Mayer considered the series

$$p=kT\sum_{s=1}^{\infty}b_s(T)z^s, \tag{6}$$

---

* The parameter, z, has been referred by Mayer as the fugacity.

which may correspond to (3). By means of (6), one may define the function $p(z)$ for complex values of z. And Mayer[9] suggested that the singularities of the analytic function obtained from (6) by the process of continuation correspond to the values of the fugacity characteristic of the phase transitions. But Mayer has neither justified the above conclusion, nor has spoken of the properties of these singularities. And he has not shown which branch of the analytic function may express the true pressure if this function is many-valued.

Katsura and Fujita[10] pointed out that the phase transitions correspond to the singularities of the function

$$p=\lim_{V\to\infty} kT\sum_{s=1}^{\infty} b_s(T, V)z^s, \tag{7}$$

rather than those of (6). Although Mayer's theory on the relation between the phase transitions and the singularities is not based on any complete proof, it seems not to have been proved by Katsura and Fujita that the first singularities of (6) and (7) do differ.

Green[3] and Rodriguez[13] have shown that the first singularity is not the point of condensation but is the point separating super-saturated vapor from liquid, but it may be plausible that this result follows from the Kirkwood approximation employed in these theories.

§ 3. The series-development method in crystal statistics

Let us consider a binary solid solution consisting of two types of atoms, A and B, of which the total potential energy is represented by the sum of the interactions of each atom with its contact neighbors. As shown in Fig. 1, let us divide the system into $l\times m\times n$ cells, each containing an A or B atom. Then, we shall denote the interactions between an AA-contact, a BB-contact, and an AB-contact by ε_{AA}, ε_{BB}, and ε_{AB}, respectively. Then the configurational partition function of the system containing r A-atoms is of the form*

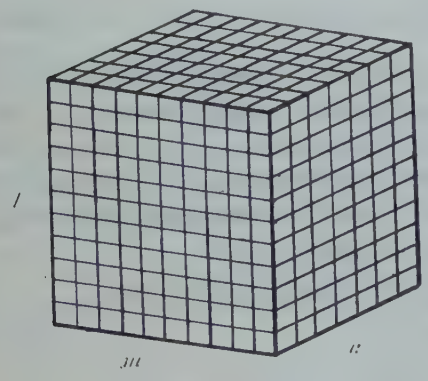

Fig. 1.

$$\Omega_r(T; l, mn)=r!\sum g(r, X; l, mn)\times \exp\{-X\Delta\varepsilon/kT\}, \tag{8}$$

where $g(r, X; l, mn)$ is the number of configurations for which the number of AB-contacts is X, and $\Delta\varepsilon$ is given by

$$\Delta\varepsilon=\varepsilon_{AB}-\frac{1}{2}(\varepsilon_{AA}+\varepsilon_{BB}).$$

---

* Strictly speaking, the configurational partition function is given by $\Omega_r(T; l, mn)\exp[-lmn\varepsilon_{BB}-r(\varepsilon_{AA}-\varepsilon_{BB})]$, the form of the grand partition function being independent of this additional factor if the active number densities, z_A and z_B are replaced by their respective effective values, $z_A\exp(\varepsilon_{BB}/kT)$ and $z_B\exp(\varepsilon_{BB}/kT)$.

The arrangements produced by only interchange between the same type of atoms are regarded as the same configuration. Denoting the effective active number densities of A and B atoms by $\bar{z}_A$ and $\bar{z}_B$ respectively, we express the grand partition function in the form

$$\bar{\Xi}(T, \bar{z}_A, \bar{z}_B; l, mn) = \bar{z}_B^{lmn} \bar{\Xi}(T, z; l, mn), \tag{9}$$

where

$$\bar{\Xi}(T, z; l, mn) = \sum_{r=0}^{lmn} \frac{z^r}{r!} \Omega_r(T; l, mn), \tag{10}$$

and

$$z = \bar{z}_A / \bar{z}_B. \tag{11}$$

As shown by Lassettre and Howe[6], if one interchanges the roles of A and B, one obtains

$$\bar{\Xi}(T, z; l, mn) = z^{lmn} \bar{\Xi}(T, 1/z; l, mn). \tag{12}$$

Since (10) is of the same form as (2), we obtain, as in the case of (4),

$$lmnb_s(T; l, mn) = \sum [\sum i r_i = s] (-)^{\Sigma r_i - 1} (\sum r_i - 1)\,! \prod_{i=1} \left[\left(\frac{\Omega_i(T; l, mn)}{i!} \right)^{r_i} \frac{1}{r_i!} \right]. \tag{13}$$

Then, as with (3), we have the relation

$$(lmn)^{-1} \ln \bar{\Xi}(T, z; l, mn) = \sum_{s=1}^{\infty} b_s(T, l, mn) z^s. \tag{14}$$

And if we introduce the function defined as

$$\exp \chi(T, z; l, mn) = [\bar{\Xi}(T, z; l, mn)]^{1/lmn}, \tag{15}$$

we obtain

$$\chi(T, z; l, mn) = \sum_{s=1}^{\infty} b_s(T; l, mn) z^s, \tag{16}$$

for z in the circle of convergence. $b_s(T; l, mn)$ is the cluster sum introduced by Fuchs[14] and Muto[15] in applying Mayer's method of clnster integrals to regular solutions. In this case the cluster sums for small values of s do not depend on l, m, n. On the other hand, Tanaka and Ogura[16], Oguchi[17] and Wakefield[18] calculated $\Omega_r(T; l, mn)$ for small r by the direct counting of complexions. Because Ω_r and b_s are related each other through (13), this method is entirely equivalent to Fuchs and Muto's one.

As in the theory of condensation, we may write, corresponding to (16),

$$\chi(T, z) = \sum_{s=1}^{\infty} b_s(T) z^s, \tag{17}$$

where

$$b_s(T) = \lim_{mn \to \infty} \lim_{l \to \infty} b_s(T; l, mn). \tag{18}$$

Furthermore, we define the following functions:

$$\chi(T, z; \infty, \infty) = \lim_{mn \to \infty} \lim_{l \to \infty} \chi(T, z; l, mn), \tag{19}$$

$$\chi(T, z; \infty, mn) = \lim_{l\to\infty} \chi(T, z; l, mn), \tag{20}$$

and

$$\chi(T, z; mn) = \sum_{s=1}^{\infty} b_s(T, mn) z^s, \tag{21}$$

where

$$b_s(T, mn) = \lim_{l\to\infty} b_s(T; l, mn). \tag{22}$$

Since we may not proceed to the limit term by term, as pointed out by Katsura and Fujita[10], (17) is not necessarily equal to (19). The same is true of (20) and (21).

According to Mayer's stand point of view, the active number density at which the phase transition occurs is given as the singularity of the function (17).

§ 4. The matrix method

The system described in the previous section consists of l layers each composed of $m \times n$ cells. Let us denote a configuration of the i'th layer by $\boldsymbol{s}_i$. In the case of solid solution, $\boldsymbol{s}_i$ corresponds to a distribution of the two types of atoms in the i'th layer, and every $\boldsymbol{s}$ assumes $2^{m\times n}$ values. Suppose the j'th and $j+1$'th layers have the distribution $\boldsymbol{s}_j$ and $\boldsymbol{s}_{j+1}$ respectively, and we denote the number of contacts of unlike atoms in the j'th layer by $X(\boldsymbol{s}_j)$ and the number of contacts of unlike atoms between the j'th and $j+1$'th by $X(\boldsymbol{s}_j, \boldsymbol{s}_{j+1})$. Then the total number of contacts of unlike atoms is given by

$$X = \sum_{j=1}^{l} X(\boldsymbol{s}_j) + \sum_{j=1}^{l} X(\boldsymbol{s}_j, \boldsymbol{s}_{j+1}). \tag{23}$$

Here we assume that the Born von Kármán boundary condition is imposed upon the system: $\boldsymbol{s}_{l+1} = \boldsymbol{s}_1$. And let $r(\boldsymbol{s}_j)$ be the number of A atom in the j'th layer at the distribution $\boldsymbol{s}_j$. Then $\bar{\Xi}(T, z; l, mn)$ given by (10) may be, according to (7) and (23), rewritten in the form

$$\bar{\Xi}(T, z; l, mn) = \sum_{\boldsymbol{s}_1} \sum_{\boldsymbol{s}_2} \cdots \sum_{\boldsymbol{s}_l} \prod_{j=1}^{l} K(\boldsymbol{s}_j, \boldsymbol{s}_{j+1}), \tag{24}$$

where

$$K(s_j, s_{j+1}) = \exp\left[\{r(\boldsymbol{s}_j) + r(\boldsymbol{s}_{j+1})\} \ln z/2 - \{X(\boldsymbol{s}_j) + X(\boldsymbol{s}_{j+1})\} \Delta\varepsilon/2kT\right]$$
$$\times \exp\{-X(\boldsymbol{s}_j, \boldsymbol{s}_{j+1}) \Delta\varepsilon/kT\}. \tag{25}$$

Lassettre and Howe[6], and Montroll[5] have shown that $\bar{\Xi}(T, z; l, mn)$ is written as

$$\bar{\Xi}(T, z; l, mn) = \sum_{\alpha=1}^{2^{m\times n}} \{\Lambda_\alpha(T, z; mn)\}^l, \tag{26}$$

where $\Lambda_\alpha(T, z; mn)$'s are $2^{m\times n}$ roots of the secular equation

$$\det |K(\alpha, \beta) - \Lambda\delta_{\alpha\beta}| = 0. \tag{27}$$

If the largest root is simple, $\chi(T, z; \infty, mn)$ defined by (15) and (20) becomes

$$\chi(T, z; \infty, mn) = (1/mn) \ln \Lambda^*(T, z; mn), \tag{28}$$

where $\Lambda^*(T, z; mn)$ is the largest of $\Lambda_\alpha(T, z; mn)$.

(27) is a plynomial of degree $2^{m\times n}$ in Λ. The coefficients of this polynomial are polynomials in z, since we can apply a suitable transformation to the matrix produced from (25), so that each element becomes a ploynomial in z. Thus $\Lambda_1(T, z; mn)$, $\Lambda_2(T, z; mn), \cdots$ form an algebraic function or a set of algebraic functions of z according as (27) is irreducible or reducible.

Since the algebraic functions cannot possess essential singular-point, the largest root of (27) must be degenerate at the active number density at which the phase transition occurs. And according to the theorem due to Frobenius, the largest root is simple and positive as far as mn is finite, because the matrix elements given by (25) are always positive, $J\varepsilon/kT$ being assumed to be finite. Thus Montroll[5] concluded that phase transitions cannot occur in the crystals infinite in only one direction.

§ 5. Singularities and degeneracy of eigenvalues

Since the coefficient of $\Lambda^{n\times m}$ in (27) is unity, any analytic function obtained from (27) has no pole, except the one at infinity, in the complex plane. Then all the singular points of the function $\Lambda(z)$ are branch-points. On the other hand, when $z=0$, the largest root of (27) is obviously simple and is equal to unity. Hence the branch of $\Lambda(z)$ which becomes unity at the origin is expressible as a power series in z about $z=0$. Let $\Lambda_1(T, z; mn)$ be the analytic function obtained from this series by the process of continuation along the positive real axis. For sufficiently small z, $\Lambda_1(T, z; mn)$ is evidently equal to $\Lambda^*(T, z; mn)$. And let z^* be the nearest singularity of $\Lambda_1(T, z; mn)$ on the positive real axis, z^* being not necessarily finite. If z^* is finite, $\Lambda_1(T, z; mn)$ has a branch-point at $z=z^*$. And, if $\Lambda^*(T, z^*; mn)=\Lambda_1(T, z^*; mn)$, the largest root is no longer simple at z^*, in contradiction with Frobenius' theorem. Then, the lower limit of the positive real z at which $\Lambda_1(T, z; mn)$ is smaller than $\Lambda^*(T, z; mn)$ must exist and smaller than z^*, and let z_1 be the value of this lower limit. This implies that $\Lambda_1(T, z; mn)$ becomes equal to other branch of the same function or some branch of other analytic function at $z=z_1<z^*$, and also contradicts with Frobenius' theorem. Hence neither z_1 nor z^* can be finite, and consequently $\Lambda^*(T, z; mn)=\Lambda_1(T, z; mn)$ for all real $z\geqq 0$. And then we see from (28) that $\chi(T, z; \infty, mn)$ represents a branch of a function which has no pole on the whole positive real axis—other branch of this function might have singularities on the positive real axis—and equal to (21) for sufficiently small z. Hence we have

$$\chi(T, z; mn)=\lim_{l\to\infty}\chi(T, z; l, mn), \tag{29}$$

if mn is finite. Here $\chi(T, z; mn)$ in the left-hand side should be understood to be the analytic function obtained from $\chi(T, z; mn)$ defined within the circle of convergence by the process of continuation along the positive real axis. Thus it has been proved that the transition from (20) to (21) is correct as far as mn is finite.

In the case of the linear chain, the equation (27) reduces to

$$\begin{vmatrix} z-\Lambda & z^{\frac{1}{2}}\exp(-\Delta\varepsilon/kT) \\ z^{\frac{1}{2}}\exp(-\Delta\varepsilon/kT) & 1-\Lambda \end{vmatrix}=0,$$

of which the largest root is given by

$$\Lambda^*(T,z\,;1)=\Lambda_1(T,z,1)=\frac{1}{2}[1+z+\{(1-z)^2+4z^2\exp(-2z\Delta\varepsilon/kT)\}^{\frac{1}{2}}]. \quad (30).$$

If $\Delta\varepsilon>0$, $\Lambda_1(T,z\,;1)$ has no zero and has a pair of branch-points at

$$z=[1-2\exp(-2\Delta\varepsilon/kT)\}\pm 2i\exp(-\Delta\varepsilon/kT)\{1-\exp(-2\Delta\varepsilon/kT)\}^{\frac{1}{2}}. \quad (31)$$

Then $\chi(T,z\,;1)$ defined by (22) is regular within the unit circle, and the radius of the circle of convergence is unity.

In the case of the two-phase separation, where $\Delta\varepsilon$ is positive, it is plausible that the radius of convergence of the series (21) may be unity as far as mn is finite. And the two-phase separation must occur at $z=1$, if it occurs, as seen from (12). If mn is sufficiently large, as in a macroscopic crystal, the change of $d\chi/dz=x/z$ at $z=1$ becomes so abrupt as experimenter observes a sharp separation into two phases. This implies that the one of the singularities on the circumference of the unit circle appears in the immediate neighborhood of the point $z=1$ on the positive real axis as mn increases.

As mn is increased, this branch-point will approach the real axis without limit. In this case, the function, $\Lambda_1(z)$, obtained as the largest root of (27) and the function $\Lambda_2(z)$, which becomes the next largest root of (27) at $z=1$ may be such that as shown in Fig. 2a. Letting mn be infinite, we obtain, from (19) and (29),

$$\chi(T,z\,;\infty,\infty)=\lim_{mn\to\infty}\chi(T,z\,;mn), \quad (32)$$

from which the thermodynamical behavior of the system of infinite extent may be derived. For the limiting function the following two cases are possible.

i) $\chi(T,z\,;\infty,\infty)$ consists of a single analytic function, at least, on the whole real axis, which has an analytic singularity at $z=1$, as shown in Fig. 2b.

ii) $\chi(T,z\,;\infty,\infty)$ consists of two different analytic functions which cross each

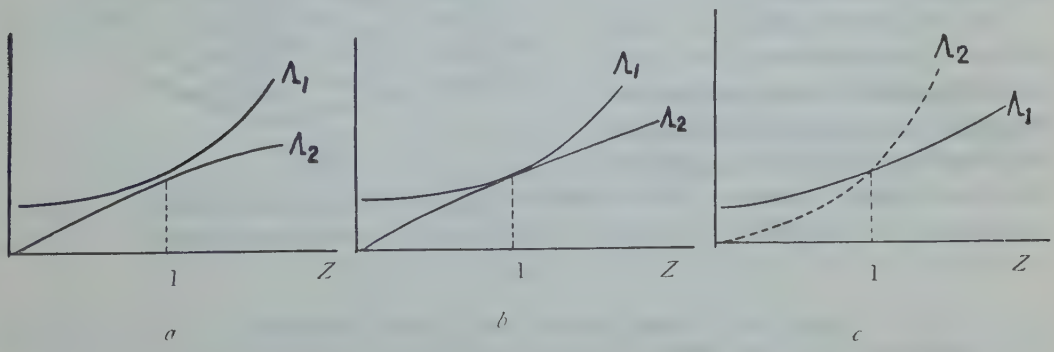

Fig. 2.

other at $z=1$ as shown in Fig. 2c*.

In the first case, $\chi(T, z; \infty, \infty)$ is identical with $\chi(T, z)$, defined as (17), at least, on the positive real axis, since both functions coincides for sufficiently small values of z. Then the first singularity of (17) is same as that of (32) on the positive real axis. And the active number density characteristic of the two-phase separation is given as the first singularity of $\chi(T, z)$ defined as (17), agreeing with Mayer's theory of condensation. And the singularity of $\chi(T, z)$ at $z=1$ must be an essential singular point, since the first derivative of χ with respect to z is finite and discontinuous at $z=1$. An example of such a function is as follows:

$$\chi(z)=z^2\{\exp(-1/z)+1\}^{-1}. \tag{33}$$

On the other hand, if ii) is the case, $\chi(T, z; \infty, \infty)$ coincides with $\chi(T, z)$ on the positive real axis only up to $z=1$. And it is possible that the first singularity of (17) and (19) may differ, as pointed out by Katsura and Fujita for the case of continuous aggregate systems.

Since the relative concentration, x, is given by $z(d\chi/dz)$, the above two cases are possible for the density of each component in binary solid solutions as a function of the active number density.

§ 6. The eigenvalue method for continuous aggregate systems

In usual from, the variables which appear in crystal statistics assume only two discrete values. In the case where molecules in each lattice site have a continuum of a possible configurations, the partition function per molecule may be calculated from one of the eigenvalues of the homogeneous integral equation instead of that of the matrix. Such a method was first applied to problems arising in statistical mechanics of linear chain of molecules by Montroll[19] and Kubo[20].

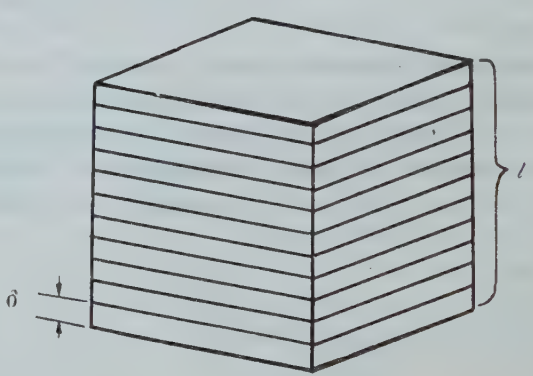

Fig. 3.

In the present paper, we shall treat the phase transition in the continuous aggregate systems, such as condensation, by means of the reduction of the problem to an eigenvalue problem of a linear integral equation. This method may be considered as a generalization of the method used by van Hove[21] in statistical mechanics of one-dimensional systems.

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* These two functions may be different branch of such an analytic function that $z=1$ is not a branch-point. And the reduciblity of the equation (27) plays no essential role in the present theory. In this point the author is indebted to Mr. K. Ikeda.

Let us consider the system in the shape of a rectangular parallelepiped with the volume V and the base of the area D. And let us divide this system into l layers, whose thickness is δ, and denote these layers by $\Delta_1, \Delta_2, \cdots, \Delta_l$ as shown in Fig. 3. The grand partition function (2) is written as

$$\Xi(T, z) = \sum_{n\geq 0} (z^n/n!) \iint\cdots\int \exp\{-U_n\{n\}/kT\}\, d\{n\}, \tag{34}$$

where $\{n\}$ is a set of coordinates of n molecules, $U_n\{n\}$ is the potential energy of n molecules at the configuration $\{n\}$, and $d\{n\}$ is the set of the volume elements of n molecules. In the configurational integral, integrals over the coordinates may be considered as a sum of integrals over each of layers

$$\Xi(T, z) = \sum_{n_1\geq 0} \sum_{n_2\geq 0} \cdots \sum_{n_l\geq 0} \frac{z_1^{n_1}}{n_1!} \frac{z_2^{n_2}}{n_2!} \cdots \frac{z_l^{n_l}}{n_l!} \int_{\Delta_1} d\{n_1\} \int_{\Delta_2} d\{n_2\} \cdots \int_{\Delta_l} d\{n_l\} \exp\left\{-\frac{U_n\{n\}}{kT}\right\}, \tag{35}$$

in which $\int d\{n\}$ for $n=0$ may be regarded as the simple multiplication by unity.

Suppose that the thickness of each layer, δ, is larger than the maximum range of intermolecular forces. Then intermolecular forces do not extend beyond immediately adjacent layers. The potential energy of the system is

$$U_n\{n\} = \frac{1}{2}\{U\{n_1\} + U\{n_l\}\} + \sum_{i=1}^{l-1} V(\{n_i\}\{n_{i+1}\}), \tag{36}$$

where

$$V(\{n_i\}, \{n_{i+1}\}) = \frac{1}{2} U\{n_i\} + U(\{n_i\}, \{n_{i+1}\}) + \frac{1}{2} U\{n_{i+1}\}, \tag{37}$$

$U\{n_i\}$ is the potential energy of n_i molecules contained in the i'th layer and $U(\{n_i\}, \{n_{i+1}\})$ is the interaction between the molecules in the i'th layer and the molecules in the $i+1$'th layer. (35) may be rewritten in the form

$$\Xi(T, z) = \sum_{n_1\geq 0} \sum_{n_2\geq 0} \cdots \sum_{n_l\geq 0} \int_{\Delta_1} d\{n_1\} \int_{\Delta_2} d\{n_2\} \cdots \int_{\Delta_l} d\{n_l\}$$

$$\times (n_1!\, n_l!)^{-1/2} z^{(n_1+n_l)/2} \exp\{-(U\{n_1\} + U\{n_l\})/kT\} \prod_{i=1}^{l-1} K(\{n_i\}, \{n_{i+1}\}), \tag{38}$$

where

$$K(\{n_i\}, \{n_{i+1}\}) = (n_i!\, n_{i+1}!)^{-1/2} z^{(n_i+n_{i+1})/2} \exp\{-V(\{n_i\}, \{n_{i+1}\})/kT\}. \tag{39}$$

If one expresses the coordinates of the molecules in Δ_i by the coordinate system with origin at the center of the i'th cell, the values of coordinates assume the same range of the values Δ. Here we introduce the notation

$$K^{(p)}(\{\lambda\}, \{\mu\}) = \sum_{\nu\geq 0} \int_{\Delta} K^{(p-1)}(\{\lambda\}, \{\nu\})\, K(\{\nu\}, \{\mu\})\, d\{\nu\}, \tag{40}$$

and

$$K^{(1)}(\{\lambda\}, \{\mu\}) = K(\{\lambda\}, \{\mu\}). \tag{41}$$

From (38), (40), and (41), we have

$$\Xi(T,z)=\sum_{n_1\geq 0}\sum_{n_l\geq 0}\int_{\Delta}\int_{\Delta}K^{(l-1)}(\{n_1\},\{n_l\})(n_1!\,n_l!)^{-1/2}z^{(n_1+n_l)/2}$$
$$\times\exp\{-(U\{n_1\}+U\{n_l\})/kT\}\,d\{n_1\}d\{n_l\}. \tag{42}$$

$K^{(p)}(\{\lambda\},\{\mu\})$ resembles the p'th iterated kernel obtained from $K(\{\lambda\},\{\mu\})$, but somewhat different from ordinary iterated kernel in the theory of linear integral equations. It may be, however, brought into the ordinary form in the manner to be described below.

If the volume of Δ is finite, the number of molecules contained in each layer cannot exceed a certain limit, say N, due to the diameter of imcompressibility of molecules. And let us consider the functions, defined in Δ, $\Psi\{N\}$, $\Psi\{N-1\}$, $\cdots$, $\Psi\{N-k\}$, $\cdots$, 1. Now we definite the function $\Phi(\{N\},\tau)$, defined in the domains Δ and τ, by

$$\Phi(\{N\},\tau)=\prod_{\alpha=1}^{N}(1-\varepsilon_\tau(\alpha))\,\Psi\{N\}+\{\varepsilon_\tau(1)/\tau\}\prod_{\alpha=2}^{N}(1-\varepsilon_\tau(\alpha))\cdot\Psi\{N-1\}$$
$$+\cdots+\prod_{\alpha=1}^{N-1}\{\varepsilon_\tau(\alpha)/\tau\}\cdot(1-\varepsilon_\tau(N))\,\Psi(1)+\prod_{\alpha=1}^{N}\{\varepsilon_\tau(\alpha)/\tau\}, \tag{43}$$

where $\varepsilon_\tau(\alpha)$ is a characteristic function of the domain τ such that

$$\varepsilon_\tau(\alpha)=\begin{cases}1 & \text{if } \alpha\text{'th molecule in } \tau,\\ 0 & \text{otherwise,}\end{cases} \tag{44}$$

τ being the normalization constant equal to the volume of this domain. If $\Psi\{n\}$ is symmetric in permutations of molecules, we have

$$\int_{\Delta+\tau}\Phi(\{N\},\tau)\,d\{N\}=\sum_{n=0}^{N}\int_{\Delta}\Psi\{n\}\,d\{n\}. \tag{45}$$

Similarly for $K(\{\lambda\},\{\mu\})$ we obtain

$$K(\{N\},\{N'\},\tau)=\sum_{k=0}^{N}\sum_{k'=0}^{N'}\prod_{\alpha=1}^{k}\{\varepsilon_\tau(\alpha)/\tau\}\prod_{\alpha=k+1}^{N}(1-\varepsilon_\tau(\alpha))\prod_{\alpha'=1'}^{k'}\{\varepsilon_\tau(\alpha)/\tau\}\prod_{\alpha'=k'+1'}^{N'}(1-\varepsilon_\tau(\alpha'))$$
$$\times K(\{N-k\},\{N'-k'\}), \tag{46}$$

where $\{N'\}$ expresses other set of N molecules than $\{N\}$, α' being the molecules of $\{N'\}$. The convention

$$K(0,0)=1$$

is used, and $\prod_{\alpha=1}^{k}\{\varepsilon_\tau(\alpha)/\tau\}$ should be regarded as unity for $k=0$. If (46) is utilized, (42), (43) and (44) are respectively expressed in the forms

$$K^{(p)}(\{N\},\{N'\},\tau)=\int_{\Delta+\tau}K^{(p-1)}(\{N\},\{N''\},\tau)\,K(\{N''\},\{N'\},\tau)\,d\{N''\}, \tag{47}$$

$$K^{(1)}(\{N\},\{N'\},\tau)=K(\{N\},\{N'\},\tau), \tag{48}$$

and

$$\Xi(T,z)=\int_{\Delta+\tau} K^{(l-1)}(\{N\},\{N'\},\tau)\,U(\{N'\},\{N\},\tau)\,d\{N\}\,d\{N'\}, \qquad (49)$$

where $U(\{N\},\{N'\},\tau)$ is the one defined by the equation like (46), in which $(\lambda!\,\mu!)^{-1/2}\,z^{(\lambda+\mu)/2}\exp\{-(U\{\lambda\}+U\{\mu\})\}/2$ appears instead of $K(\{\lambda\},\{\mu\})$.

Since $K^{(l-1)}(\{N\},\{N'\},\tau)$ increases with l, and $U(\{N\},\{N'\},\tau)$ becomes asymptotically independent of $\{N\}$, $\{N'\}$, one obtains, in the limit of increasing l, from (49)

$$\Lambda(T,z;D)=\lim_{l\to\infty}[\Xi(T,z)]^{1/l}=\lim_{l\to\infty}[K^{(l-1)}(\{N\},\{N'\},\tau)]^{1/l}, \qquad (50)$$

in which $\Lambda(T,z;D)$ corresponds to $\Lambda^*(T,z;m\mu)$ in (29), as seen from (15), (20) and (29).

Now let us consider the power series in Λ defined by

$$k(\{N\},\{N'\},\tau)=\sum_{p=1}^{\infty} K^{(p)}(\{N\},\{N'\},\tau)\,\Lambda^p, \qquad (51)$$

the radius of the circle of convergence of this series is $\Lambda(T,z;D)$ given by (50) according to Cauchy and Hadamard's theorem[22]. On the other hand, (51) is Neumann's series in the theory of Fredholm's integral equation. And according to Fredholm's theorem[22], the radius of the circle of convergence of (51) is equal to the eigenvalues with the minimum absolute value of the equation. This eigenvalue is given as the root with minimum absolute value of the equation

$$D(\lambda)=0, \qquad (52)$$

where $D(\lambda)$ is

$$D(\lambda)=-\lambda\int_{\Delta+\tau} K(\{N\},\{N\},\tau)\,d\{N\}$$
$$+\frac{\lambda^2}{2}\iint_{\Delta+\tau}\begin{vmatrix} K(\{N\},\{N\},\tau) & K(\{N\},\{N'\},\tau) \\ K(\{N'\},\{N\},\tau) & K(\{N'\},\{N'\},\tau)\end{vmatrix} d\{N\}\,d\{N'\}\cdots . \qquad (53)$$

A set of the roots of (52) may be represented by an analytic function or a set of analytic functions of z, as in the case of the set of roots of (27). The phase transition in continuous aggregate system may corresponds to the degeneracy of the smallest root of (52). And this root, $\Lambda^*(T,z;D)$, may be expressed in the power series in z. And one sees from (1), (50), and (51) that the pressure is given by

$$p/kT=\lim_{D\to\infty}\ln\Lambda^*(T,z;D)/\delta D. \qquad (54)$$

And for sufficiently small values of z (54) may agree with (6). Hence the same discussion as in the case of crystal statistics is applied to the continuous case. And Mayer's theory is correct if the value of the active number density for which the smallest root of (52) degenerates is the analytic singular point of the function $\Lambda^*(T,z;D)$, and otherwise the first singularity of (6) may differ from that of (7), as stated in the objection proposed by Katsura and Fujita.

The above theory is somewhat like Mayer's simplified caricature of phase transition[23],

though in Mayer's treatment the value of the active number density characteristic of phase transition appears as the smallest eigenvalue of the integral equation.

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References

1) J. G. Kirkwood, J Chem. Phys. **3** (1935), 300.
2) J. Yvon, Actualités Scientifiques et Industrielles (Herman et Cie, Paris, 1935), p. 203.
3) M. Born and H. S. Green, Proc. Roy. Soc. **A 188** (1946), 10; H. S. Green, Proc. Roy. Soc. **A 189** (1947), 103.
4) H. A. Kramers and G. H. Wannier, Phys. Rev. **60** (1941), 252, 263.
5) E. Montroll, J. Chem. Phys. **9** (1941), 706; **10** (1942), 61.
6) E. N. Lassettre and J. P. Howe, J. Chem. Phys. **9** (1941), 747, 801.
7) L. Onsager, Phys. Rev. **65** (1944), 117.
8) J. E. Mayer, J. Chem. Phys. **5** (1937), 67; **6** (1938), 87, 101; J. E. Mayer and M. G. Mayer, *Statistical Mechanics* (New York, 1940), Chapters 13 and 14.
9) J. E. Mayer, J. Chem. Phys. **10** (1942), 629.
10) S. Katsura and H. Fujita, J. Chem. Phys. **19** (1951), 795; Prog. Theor. Phys. **6** (1951), 498.
11) S. Ono, J. Chem. Phys. **19** (1951), 504.
12) B. Kahn and G. E. Uhlenbeck, Physica **5** (1938), 388.
13) A. E. Rodriguez, Proc. Roy. Soc. **A 196** (1949), 73.
14) K. Fuchs, Proc. Roy. Soc. **A 179** (1942), 73.
15) Y. Muto, J. Phys.-Math. Soc. Japan (in Japanese) **17** (1943), 86; J. Chem. Phys. **16** (1938), 519, 524.
16) T. Tanaka and K. Ogura, Busseiron Kenkyu (in Japanese) No. 15 (1949), 29; T. Tanaka, Busseiron Kenkyu (in Japanese) No. 20 (1949), 55, 102; T. Tanaka, H. Katsumori and S. Toshima, Prog. Theor. Phys. **6** (1951), 17.
17) T. Oguchi, J. Phys. Soc. Japan **6** (1951), 27, 31.
18) A. J. Wakefield, Proc. Cambridge Phil. Soc. **47** (1951), 419.
19) E. Montroll, Annals of Mathematical Statistics **18** (1947), 18.
20) R. Kubo, J. Phys. Soc. Japan **2** (1947), 47.
21) L. Van Hove, Physica **16** (1950), 137.
22) E. Goursat, *Cours d'analyse mathematique*, Vol. 3 (Paris, 1923), Chapters 13 and 14.
23) J. E. Mayer, J. Chem. Phys. **15** (1947), 187.

Note added in proof. Recently C. N. Yang and T. D. Lee (private communications to the author) have shown that all zeros of (10) are on the unit circle with the centre at the origin, and the series (16) converges uniformly at every interior point of this circle, if $\Delta\varepsilon$ is positive. Consequently, in the two-phase-separation case of crystal statistics, (32) is certainly regular in the half-open interval $0 \leqq z < 1$ on the positive real axis, as considered in the present paper.

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Interaction of μ Meson with Matter, II

Spontaneous Decay of Negative μ Meson

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The negative μ meson decay from the bound state around the nucleus has been worked out. The characteristic differences of the energy spectra of decay electrons and the decay life time of negative μ meson in comparison with those of positive μ meson have been pointed out for a number of mass values of neutral particle μ_0=0, 20m, 40m and several forms of couplings of the decay process. The possibilities to observe such characteristics of negative μ meson have been discussed briefly.

§ 1. Introduction

As is well-known both experimentally and theoretically, the behaviour of slow negative μ meson in matter has been described as consisting of two steps: one in which the negative μ meson is captured in the Bohr orbit with the radius of order of 10^{-12}cm after losing its energy mainly through the ionization loss; second, a step in which the spontaneous and induced decays of μ meson take place in competitive manner, the latter of which is induced by the typically nuclear interactions with the nearby nucleons. The present paper will be primarily concerned with the detailed description of one in the second step, i.e., the spontaneous decay of negative μ meson. According to Fermi and Teller[1], the average time required to slow a μ meson from the relativistic 10^8 volts to 2000 ev. is estimated to be about 10^{-9} to 10^{-10} second in condensed matter, or 10^3 times as long in air, while that needed for the μ meson to jump down into the Bohr orbit of the lowest state from the mentioned energy of 2000 ev. to be about 10^{-13} to 10^{-14} second in condensed matter or 10^4 times as long in normal air, in which the various kinds of processes, i.e., the ionization loss, the Auger transition and the radiative one take place.[2] These times for the overall processes of stopping of negative μ mesons in matter is remarkably short compared with the spontaneous life time of about $2\cdot10^{-6}$ second, so that the ultimate disappearance of negative μ meson is governed by the balance between the spontaneous and induced decays[3] both from the lowest quantized state around the nucleus. On the other hand, the spontaneous decay of positive μ meson may be considered to take place from its free state of practically zero velocity after losing its energy mainly through the ionization loss in matter.

According to the theoretical investigation of Tiomno and Wheeler[4], the energy spectrum of electrons from μ meson decay on the basis of three particles disintegration hypothesis seems to be in qualitative agreement with the present experimental evidences of Steinberger,[5] Leighton, Anderson, Seriff[6] and Sagane.[7] Since Tiomno and Wheeler have worked out

the decay process from μ meson at rest, their results may be considered to be approximately valid for positive μ meson in view of the stopping mechanism of μ meson in matter mentioned above. In the present paper the similar decay process of negative μ meson from the K-orbit around the nucleus has been worked out theoretically on the purely phenomenological grounds similar to the case of Tiomno and Wheeler, thus being independent of deeper question of meson theory, and the characteristic differences between energy spectra of decay-electrons and positrons have been pointed out. The possibility to observe such differences in the electron energy spectra will not be hopeless in view of the remarkably large intensity of artificially produced mesons now available in the laboratories. The effect upon spontaneous decay life time of the binding around the nucleus has been discussed by using our numerical results.

In the course of preparing our manuscript of the present paper, it has come to our attention that Porter and Primakoff[8] have worked theoretically the similar problem of negative μ meson decay from the Bohr orbit by the use of the charge retention and asymmetrical charge processes, the emitted neutral particle μ_0 being assumed to be neutrino. Their results about the energy spectra of electrons are quite similar to ours although, in our case, the mass of one of the neutral particles has been assumed not to be zero in order to obtain some knowledge of the effect on the mentioned energy spectra and life time of the mass value of a neutral particle, with the expectation that the detailed analysis of the energy spectra of electrons from μ meson decay will lead to the possible determination of the mass of the neutral particle on a similar way to the case of the β decay process.

§ 2. Hamiltonian for the coupling

According to Tiomno and Wheeler,[9] it has been supposed here to consider μ meson decay as a three particle process of the type

$$\mu^- \rightarrow \mu_0 + \nu + e, \tag{1}$$

where μ^-, μ_0, e and ν represent a negative μ meson, a neutral particle, an electron and a neutrino respectively. In treating the decay process we shall consider the μ^- and μ_0 meson both to have spin $=1/2$. In the mathematical formulation of μ meson decay, as of the β decay, it is convenient to adopt a description in which the process appears as the disappearance of two particles and the reappearance of two other particles. We, therefore, may represent the process (1) in the form $\mu^- + \bar{\nu}$ (neutrino in the negative energy state) $\rightarrow \mu_0 + e$, thus the fundamental positive energy particles being considered as the entities μ^- and e; which situation is essentially required for the reasonable description of the bound state of μ^- meson in our case.

The perturbation Hamiltonians responsible for the mentioned decay process are written, in a similar way to that of Tiomno and Wheeler, as

$$H_s = g_s \beta_H \beta_L (\tau_H \tau_L + \tau_H^* \tau_L^*) \ \delta(\vec{x}_H - \vec{x}_L), \qquad \text{(scalar coupling)} \tag{2}$$

$$H_v = g_v(1-\vec{\alpha}_H\vec{\alpha}_L)(\tau_H\tau_L+\tau_H^*\tau_L^*)\ \delta(\vec{x}_H-\vec{x}_L), \quad \text{(vector coupling)} \qquad (3)$$

$$H_t = 3^{-1/2}\, g_t(\beta_H\vec{\sigma}_H\cdot\beta_L\vec{\sigma}_L+\beta_H\vec{\alpha}_H\cdot\beta_L\vec{\alpha}_L)\cdot$$
$$\cdot(\tau_H\tau_L+\tau_H^*\tau_L^*)\ \delta(\vec{x}_H-\vec{x}_L), \quad \text{(tensor coupling)} \qquad (4)$$

$$H_{pv} = 3^{-1/2} g_{pv}(\vec{\sigma}_H\vec{\sigma}_L-\gamma_H^5\gamma_L^5)(\tau_H\tau_L+\tau_H^*\tau_L^*)\cdot$$
$$\delta(\vec{x}_H-\vec{x}_L), \quad \text{(pseudo-vector coupling)} \qquad (5)$$

$$H_{ps} = g_{ps}(\beta_H\gamma_H^5\cdot\beta_L\gamma_L^5)(\tau_H\tau_L+\tau_H^*\tau_L^*)\cdot$$
$$\cdot\delta(\vec{x}_H-\vec{x}_L), \quad \text{(pseudo-scalar coupling)} \qquad (6)$$

where the subscripts H and L refer to the particles μ^-, μ_0 and e, ν respectively. The operators τ_L and τ_L^* change an electron into a neutrino, and conversely. Similarly the operators τ_H and τ_H^* produce the changes $\mu^-\to\mu_0$ and $\mu_0\to\mu^-$ in the case of meson decay. α and β denote the usual Dirac operators, out of which may be built up $\sigma_x=i\alpha_y\alpha_z$ and $\gamma^5=i\alpha_x\alpha_y\alpha_z$. The quantities g will be called the coupling constants, having the dimension of erg. cm^3, and the factor $3^{-1/2}$ is introduced in the tensor and pseudo-vector cases in order to give the same value to the coupling constant of ordinary β-decay theory in all the four cases. According to Wheeler, g in μ decay becomes of the order of about 10^{-49} erg. cm^3.

§ 3. Transition probabilities

For the case of μ^+ meson decay from a free state, the final states in the transition will be restricted in accordance with both conservation laws of energies and momenta of the concerned particles, while, for the μ^- meson decay from a bound state under consideration, by the energy conservation law alone since the recoil of a nucleus, around which μ^- meson is bound, may be allowed to be neglected on account of its large mass.

The conservation of energy in our case requires

$$E_\mu = E_e + E_\nu + E_0, \qquad (7)$$

where E_μ, E_e, E_ν and E_0 denote the energies of a bound μ^- meson, an electron, a neutrino and a neutral particle respectively.

The transition probability P may be written, according to the general theory of quantum mechanics, as

$$P = \frac{2\pi}{\hbar}\cdot\sum|(i|H|f)|^2\rho_E dE\ \delta(E_\mu-E), \qquad (8)$$

in which $(i|H|f)$ represents a transition matrix element corresponding to (2)$\sim$(6), ρ_E a state density of the final states, $\sum|(i|H|f)|^2$ the square of the matrix element for the transition, averaged over the spin of the original meson and summed over all directions of spin of the three products of decay, and the remaining quantities have the usual meanings.

The transition matrix element is given by

$$(i|H|f)=\int\int\psi_0^*\psi_e^*H\,\psi_-\psi_\nu\;d\vec{r}_H\cdot d\vec{r}_L. \tag{9}$$

Here ψ_0, ψ_ν and ψ_e represent Dirac's wave functions[10] of a free neutral particle, a free neutrino and a free electron respectively. The effect of a nuclear charge on the emitted electron may be neglected on account of the extremely large kinetic energy (10～50 Mev) in comparison with that of β decay electron. ψ_- denotes Dirac wave function of a negative μ^- meson in the K-orbit around the nucleus, namely,[11]

$$\psi_-=\frac{1}{\sqrt{4\pi}}\begin{pmatrix} if(r)\ \cos\theta \\ if(r)\ \sin\theta e^{i\varphi} \\ g(r) \\ 0 \end{pmatrix}\text{or}\ \frac{1}{\sqrt{4\pi}}\begin{pmatrix} -if(r)\ \sin\theta e^{-i\varphi} \\ if(r)\ \cos\theta \\ 0 \\ -g(r) \end{pmatrix}, \tag{10}$$

corresponding to each of two spin states of μ^- meson respectively. $g(r)$ and $f(r)$ are the radial wave functions of large and small components respectively, the explicit forms of which are written as

$$f(r)=-\sqrt{\frac{\lambda(1-\varepsilon)}{\Gamma(2\varepsilon+1)}}(2\lambda r)^{\varepsilon}e^{-\lambda r}/r,\quad g(r)=-\sqrt{\frac{1+\varepsilon}{1-\varepsilon}}f(r), \tag{11}$$

$$\varepsilon=\sqrt{1-\alpha^2Z^2},\qquad \lambda=\mu c/\hbar. \tag{12}$$

cZ expresses a nuclear charge, α a fine structure constant, μ a mass of negative μ meson, c light velocity, $\hbar$ Planck's constant divided by 2π and $\Gamma(x)$ Gamma function of x.

When we put

$$I=\sum|(i|H|f)|^2, \tag{13}$$

it follows, after some process of computations,

$$I_s=\frac{1}{2}\frac{g_s^2}{V^3}\left\{1+\frac{c^2(\vec{p}_e\cdot\vec{p}_\nu)}{E_eE_\nu}\right\}\cdot\left\{(1+\frac{\mu_0c^2}{E_0})G^2k^2+2\frac{(\vec{k}c\cdot\vec{p}_0)}{E_0}FGk+(1-\frac{\mu_0c^2}{E_0})F^2k^2\right\}, \tag{14,1}$$

$$\begin{aligned} I_v=\frac{g_v^2}{V^3}\Big\{&\Big[2-\frac{\mu_0c^2}{E_0}\Big(1+\frac{c^2(\vec{p}_e\cdot\vec{p}_\nu)}{E_eE_\nu}\Big)+\frac{c^2(\vec{p}_\nu\cdot\vec{p}_0)}{E_0E_\nu}-\frac{c^2(\vec{p}_e\cdot\vec{p}_0)}{E_0E_e}\Big]G^2k^2 \\ &+2\Big[\frac{(\vec{k}\cdot c\vec{p}_e)}{E_e}-\frac{(\vec{k}\cdot c\vec{p}_\nu)}{E_\nu}+\frac{c^3(\vec{p}_0\cdot\vec{p}_\nu)(\vec{k}\cdot\vec{p}_e)+c^3(\vec{p}_0\cdot\vec{p}_e)(\vec{k}\cdot\vec{p}_\nu)}{E_0E_eE_\nu}\Big]FGk \\ &+\Big[2+\frac{\mu_0c^2}{E_e}\Big(1+\frac{c^2(\vec{p}_e\cdot\vec{p}_\nu)}{E_eE_\nu}\Big)+\frac{c^2(\vec{p}_\nu\cdot\vec{p}_0)}{E_0E_\nu}-\frac{c^2(\vec{p}_e\cdot\vec{p}_0)}{E_eE_0}\Big]F^2k^2\Big\}, \end{aligned} \tag{14,2}$$

$$\begin{aligned} I_t=\frac{1}{3}\frac{g_t^2}{V^3}\Big\{&\Big[3-\frac{c^2(\vec{p}_e\cdot\vec{p}_\nu)}{E_eE_\nu}-2\frac{c^2(\vec{p}_0\cdot\vec{p}_e)}{E_0E_e}+2\frac{c^2(\vec{p}_\nu\cdot\vec{p}_0)}{E_\nu E_0}\Big](F^2+G^2)k^2+2\Big[\frac{c(\vec{p}_e\cdot\vec{k})}{E_e} \\ &-\frac{c(\vec{p}_\nu\cdot\vec{k})}{E_\nu}-\frac{c(\vec{p}_0\cdot\vec{k})}{E_0}-\frac{1}{2}\frac{c^3(\vec{p}_0\cdot\vec{k})(\vec{p}_e\cdot\vec{p}_\nu)}{E_0E_eE_\nu} \\ &+2\cdot\frac{c^3(\vec{p}_e\cdot\vec{k})(\vec{p}_0\cdot\vec{p}_\nu)+c^3(\vec{p}_\nu\cdot\vec{k})(\vec{p}_0\cdot\vec{p}_e)}{E_0E_eE_\nu}\Big]FGk\Big\}, \end{aligned} \tag{14,3}$$

$$I_{pv}=\frac{1}{3}g^2_{pv}/g^2_v\cdot I_v(\mu_o\rightarrow-\mu_o), \tag{14,4}$$

$$I_{ps}=g^2_{ps}/g^2_s\cdot I_s(\mu_0\rightarrow-\mu_0), \tag{14,5}$$

where $\vec{p}_e$, $\vec{p}_\nu$ and $\vec{p}_0$ denote the momenta of an electron, a neutrino and a neutral particle respectively. μ_0 is the mass of neutral particle and l^3 the normalization volume. Further, we have

$$\hbar\vec{k}=\vec{p}_\nu-\vec{p}_0-\vec{p}_e, \tag{15}$$

$$F=\sqrt{\frac{1-\varepsilon}{1+\varepsilon}}\cdot A\int_0^\infty r^\varepsilon\left(\frac{\sin kr}{kr}-\cos kr\right)e^{-\lambda r}dr, \tag{16}$$

$$G=A\int_0^\infty r^\varepsilon e^{-\lambda r}\sin kr\ dr, \tag{17}$$

$$A=(2\lambda)^\varepsilon/k^2\cdot\sqrt{4\pi\lambda\,(1+\varepsilon)/\Gamma(2\varepsilon+1)}. \tag{18}$$

For the case of $(\alpha Z)^2\langle\langle 1$, we get readily

$$F\approx\sqrt{2\pi\lambda}\cdot 2\lambda(\alpha Z)/(k^2+\lambda^2)^2, \tag{16}'$$

$$G\approx\sqrt{2\pi\lambda}\cdot(2\lambda)^2/k(k^2+\lambda^2)^2. \tag{17}'$$

As seen in (16), (17), (16)′ and (17)′ F becomes smaller than G due to a factor αZ involved in F, on account of which F^2-terms contained in I ((14,1)∼(14,5)) are allowed to be dropped compared with G^2-and FG-terms in our computations.

In order to obtain the probability per second of a negative μ decay process in which the electron emerges in the energy interval E_e to E_e+dE_e, we have to carry out the integrations over $\vec{p}_\nu$ and $\vec{p}_0$ of (8) after substituting (14,1)∼(14,5), (16)′∼(17)′ into (8). In such manipulation we have made use of the following change of variables;

$$\vec{\alpha}=\vec{p}_\nu-\vec{p}_0,\quad \vec{\beta}=\vec{p}_\nu, \tag{18}$$

which leads to

$$\rho_E=\rho_\beta\frac{d\beta}{dE}=\frac{V^3}{(2\pi\hbar c)^9}\cdot\frac{W-\beta}{W-Z_\beta\alpha}\alpha^2\,d\alpha\,\beta^2\,d\beta\,d\Omega_\alpha\,d\Omega_\beta\,d\Omega_e\,p_e^2\,dp_e, \tag{19}$$

$$W=(E_\mu-E_e)/c,\ \beta_0=W-E_0/c,\ Z_\beta=\cos\theta_\beta\ . \tag{20}$$

Here $d\Omega_\alpha$, $d\Omega_\beta$ and $d\Omega_e$ represent the solid angles of $\vec{\alpha}$, $\vec{\beta}$ and $\vec{p}_e$ respectively. The integration over β of δ-function in (8) is equivalent to putting β_0 for β in the integrand of (8).

After some process of manipulation, we get finally, for the mentioned transition probability P,

$$P=\frac{2\pi}{\hbar}\cdot\frac{(2\lambda)^4}{(2\pi\hbar c)^9}\cdot(4\pi\lambda)\cdot g_i^2\cdot f_i\,dE_e, \tag{21}$$

$$(g_i=g_s, g_v, g_t, g_{pv}, g_{ps};\ f_i=f_s, f_v, f_t, f_{pv}, f_{ps})$$

$$f_s=\frac{1}{2}\left(f_{s,G^2}+\frac{1}{\mu c^2}\cdot f_{s,FG}\right), \tag{22,1}$$

$$f_v=f_{v,G^2}+\frac{1}{\mu c^2}\cdot f_{v,FG}, \tag{22,2}$$

$$f_t=\frac{1}{3}\left(f_{t,G^2}+\frac{1}{\mu c^2}\cdot f_{t,FG}\right), \tag{22,3}$$

$$f_{pv}=\frac{1}{3}\left(f_{pv,G^2}+\frac{1}{\mu c^2}f_{pv,FG}\right), \tag{22,4}$$

$$f_{ps}=\frac{1}{2}\left(f_{ps,G^2}+\frac{1}{\mu c^2}f_{ps,FG}\right), \tag{22,5}$$

where f_{i,G^2} or $f_{i,FG}$ represents each of the contributions from G^2- or FG-term respectively. The general form of the integrals involved in f_{i,G^2} and $f_{i,FG}$ becomes

$$\int d\vec{p}_e\, d\vec{p}_\nu\, d\Omega_e \frac{f(\vec{p}_e,\vec{p}_\nu,\vec{p}_0)}{(k'^2+\lambda'^2)}=\int d\vec{\alpha}\int d\Omega_e\int d\Omega_\alpha \frac{\beta_0^2}{(\alpha^2+p_e^2-2(\vec{p}\cdot\vec{\alpha}_e)+\lambda'^2)}\cdot\frac{W-\beta_0}{W-Z_{30}\alpha}\cdot f(\vec{\alpha},\vec{\beta}_0,\vec{p}_e), \tag{23}$$

$$\lambda'=\hbar\lambda, \qquad k'=\hbar k. \tag{23'}$$

For carrying through the evaluation of (23), we have manipulated first $\int d\Omega_\beta\cdots\cdots$ with a polar axis along the direction of $\vec{\alpha}$, then $\int d\Omega_\alpha$ with a polar axis parallel to $\vec{p}_e$ and finally $\int d\Omega_e\cdots\cdots$. After some process of the elementary but rather tedious computations, we obtain finally

$$\begin{aligned}f_{s,G^2}=2(2\pi)^3\sum_{\varepsilon=-1}^{1}\Big\{&(W+\mu_0 c)\xi_3^2-\xi_3^3+\frac{1}{4E_e}\{(\mu_0 c+W)[(\xi_3^1-2W\xi_3^2-(W^2-\mu_0^2c^2)\zeta_3^1)\cdot\\ &\cdot(p_e^2+\lambda'^2)+(\eta_3^1+2W\xi_3^2-(W^2-\mu^2{}_0c^2)\xi_3^1)-(\xi_2^1+2W\zeta_2^2-(W^2-\mu^2{}_0c^2)\zeta_2^1)]\\ &-[(\xi_3^2+2W\zeta_3^3-(W^2-\mu_0^2c^2)\zeta_3^2)(p_e^2+\lambda'^2)+(\eta_3^2+2W\xi_3^3-(W^2-\mu_0^2c^2)\xi_3^2)\\ &-(\xi_2^3+2W\zeta_2^3-(W^2-\mu_0^2c^2)\zeta_2^2)]\}\Big\},\end{aligned} \tag{24,1}$$

$$f_{ps,G^2}=f_{s,G^2}(\mu_0\to-\mu_0), \tag{24,2}$$

$$f_{v,G^2}=f_{ps,G^2}+f_{e,G^2}, \tag{24,3}$$

$$f_{pv,G^2}=f_{v,G^2}(\mu_0\to-\mu_0), \tag{24,4}$$

$$f_{t,G^2}=(f_{s,G^2}+f_{ps,G^2})/2+2f_{e,G^2}, \tag{24,5}$$

$$\begin{aligned}f_{e,G^2}=2(2\pi)^3\sum_{\varepsilon=-1}^{1}\Big\{&W\xi_3^2+(W^2-\mu_0^2c^2)/2\cdot\xi_3^1-\eta_3^1/2-W\xi_3^2+\frac{1}{2E_e}\{(p_e^2+\lambda'^2)\xi_3^2+\eta_3^2\\ &-\xi_2^2-\frac{W}{2}[(\xi_3^1+2W\zeta_3^2-(W^2-\mu^2{}_0c^2)\zeta_3^1)(p_e^2+\lambda'^2)+(\eta_3^1+2W\xi_3^2-(W^2-\mu_0^2c^2)\xi_3^1)\end{aligned}$$

$$-(\xi_2^1+2W\zeta_2^2-(W^2-\mu_0^2c^2)\zeta_2^1)]\}\Big\}, \qquad (24,6)$$

$$f_{s,FG}=2(2\pi)^3\sum_{\varepsilon=-1}^{1}\Big\{W\xi_3^3-(W^2-\mu_0^2c^2)/2\cdot\xi_3^2+\eta_3^2/2-\eta_3^2-\frac{1}{4}\{(\xi_3^2+2W\zeta_3^3$$

$$-(W^2-\mu_0^2c^2)\zeta_3^2)(p_e^2+\lambda'^2)+(\eta_3^2+2W\xi_3^3-(W^2-\mu_0^2c^2)\xi_3^2)-(\xi_2^3+2W\zeta_2^3$$

$$-(W^2-\mu_0^2c^2)\zeta_2^2)\}+\frac{1}{2}\{(p_e^2+\lambda'^2)\xi_3^2+\eta_3^2-\xi_2^2\}+\frac{1}{2E_e^2}W^2((p_e^2+\lambda'^2)\zeta_3^3-\zeta_2^3+\xi_3^3)$$

$$-W((W^2-\mu_0^2c^2)\cdot((p_e^2+\lambda'^2)\zeta_3^2-\zeta_2^2+\xi_3^2)+\frac{1}{4}(W^2-\mu_0^2c^2)^2((p_e^2+\lambda'^2)\zeta_3^1-\zeta_2^1+\xi_3^1)$$

$$+W(p_e^2+\lambda'^2)\xi_3^2-\xi_2^2+\eta_3^2)-\frac{1}{2}(W^2-\mu_0^2c^2)((p_e^2+\lambda'^2)\xi_3^1-\xi_2^1+\eta_3^1)+\frac{1}{4}((p_e^2+\lambda'^2)\eta_3^1$$

$$-\eta_2^1+\Theta_3^1)-W((p_e^2+\lambda'^2)\xi_3^2-\xi_2^2+\eta_3^2)+\frac{1}{2}(W^2-\mu_0^2c^2)((p_e^2+\lambda'^2)\xi_3^1-\xi_2^1+\eta_3^1)$$

$$-\frac{1}{2}((p_e^2+\lambda'^2)\eta_3^1-\eta_2^1+\Theta_3^1)-3W^2(\frac{1}{4}\Phi_1^3-\frac{1}{2}(p_e^2+\lambda'^2)\Phi_2^3+\frac{1}{4}(p_e^2+\lambda'^2)^2\Phi_3^3)$$

$$+3W(W^2-\mu_0^2c^2)(\frac{1}{4}\Phi_1^2-\frac{1}{2}(p_e^2+\lambda'^2)\Phi_2^2+\frac{1}{4}(p_e^2+\lambda'^2)\Phi_3^2)-\frac{3}{4}(W^2-\mu_0^2c^2)^2\cdot$$

$$(\frac{1}{4}\Phi_1^1-\frac{1}{2}(p_e^2+\lambda'^2)\Phi_2^1+\frac{1}{4}(p_e^2+\lambda'^2)^2\Phi_3^1)+\frac{1}{4}\zeta_1^3-\frac{1}{2}(p_e^2+\lambda'^2-3W^2)\zeta_2^3$$

$$-\frac{1}{4}(2W^2(3\lambda'^2+p_e^2)-(p_e^2+\lambda'^2)^2)\zeta_3^3-\frac{3}{4}W\zeta_1^2+\frac{3}{2}W\cdot(p_e^2+\lambda'^2-W^2+\mu_0^2c^2)\zeta_2^2$$

$$-\frac{1}{4}W(3(p_e^2+\lambda'^2)^2-2(W^2-\mu_0^2c^2)(p_e^2+3\lambda'^2))\zeta_3^2-\frac{3}{8}(W^2-\mu_0^2c^2)((2p_e^2+2\lambda'^2$$

$$-W^2+\mu_0^2c^2)\zeta_2^1-\zeta_1^1)+\frac{1}{8}(W^2-\mu_0^2c^2)\{3(p_e^2+\lambda'^2)^2-(W^2-\mu_0^2c^2)(p_e^2+3\lambda'^2)\}\zeta_3^1$$

$$-\frac{1}{2}\xi_2^3-\frac{1}{4}(3W^2+2p_e^2-2\lambda'^2)\xi_3^3+\frac{3}{2}W\xi_2^2-\frac{1}{4}W(6\lambda'^2+2p_e^2-3W^2+3\mu_0^2c^2)\xi_3^2-\frac{3}{16}\xi_1^1$$

$$-\frac{3}{8}(2W^2-2\mu_0^2c^2-p_e^2-\lambda'^2)\xi_2-\frac{1}{16}\{3(p_e^2+\lambda'^2)^2-4(W^2-\mu_0^2c^2)(p_e^2+3\lambda'^2)+3(W^2$$

$$-\mu_0^2c^2)^2\}\xi_3^1+\frac{1}{4}\eta_3^3-\frac{3}{4}W\eta_3^2-\frac{1}{8}(3\lambda'^2+p_e^2-3W^2+3\mu_0^2c^2)\eta_3^1+\frac{3}{8}\eta_2^1-\frac{3}{16}\Theta_3^1-\frac{1}{4}(W^2$$

$$-\mu_0^2c^2)\zeta_1^1+\frac{1}{2}(W^2-\mu_0^2c^2)(p_e^2+\lambda'^2)\zeta_2^1-\frac{1}{4}(W^2-\mu_0^2c^2)\cdot(p_e^2+\lambda'^2)^2\zeta_3^1+\frac{1}{2}W\zeta_1^2-W(p_e^2$$

$$+\lambda'^2)\zeta_2^2+\frac{1}{2}W(p_e^2+\lambda'^2)^2\zeta_3^2+\frac{1}{4}\xi_1^1-\frac{1}{2}(p_e^2+\lambda'^2-W^2+\mu_0c^2)\xi_2^1+\frac{1}{4}(p_e^2+\lambda'^2)(p_e^2$$

$$+\lambda'^2-2W^2+2\mu_0^2c^2)\xi_3^1-W\xi_2^2+W(p_e^2+\lambda'^2)\xi_3^2-\frac{1}{2}\eta_2^1+\frac{1}{4}(2p_e^2+2\lambda'^2-W^2+\mu_0^2c^2)\eta_3^1$$

$$+\frac{1}{2}W\eta_3^2+\frac{1}{4}\theta_3^1]\Big\}, \tag{25,1}$$

$$f_{ps,\,FG}=f_{s,\,FG}(\mu_0\to-\mu_0), \tag{25,2}$$

$$f_{v,\,FG}=f_{ps,\,FG}+f_{c,\,FG}, \tag{25,3}$$

$$f_{t,\,FG}=(f_{s,\,FG}+f_{ps,FG})/2+2f_{c,\,FG}, \tag{25,4}$$

$$f_{pv,FG}=f_{v,FG}\,(\mu_0\to-\mu_0), \tag{25,5}$$

$$f_{c,FG}=(2\pi)^3\sum_{\varepsilon=-1}^{1}\Big\{\frac{1}{E_e}[(p_e^2+\lambda'^2)(W\xi_3^2-\xi_3^3)-(W\xi_2^2-\xi_2^3)+(W\eta_3^2-\eta_3^3)]$$

$$+\frac{1}{E_e}[(p_e^2+\lambda'^2)\xi_3^3+\eta_3^3-\xi_2^3-W(p_e^2+\lambda'^2)\xi_3^2+\frac{1}{2}(p_e^2+\lambda'^2)(W^2-\mu_0^2c^2)\xi_3^1$$

$$-\frac{1}{2}(p_e^2+\lambda'^2)\eta_3^1-W\eta_3^2+\frac{1}{2}(W^2-\mu_0^2c^2)\eta_3^1-\frac{1}{2}\theta_3^1+W\xi_2^2$$

$$-\frac{1}{2}(W^2-\mu_0^2c^2)\xi_2^1+\frac{1}{2}\eta_2^1$$

$$-p_e^2((W^2-\mu_0^2c^2)\xi_3^1-\eta_3^1-2W\xi_3^2)$$

$$-2p_e^2W\xi_3^2]\Big\}. \tag{25,6}$$

Here the quantities of ξ_n^m, η_n^m, ζ_n^m, θ_n^m and Φ_n^m are expressed by

$$\xi_n^m=\frac{1}{m}\int\frac{1}{-\varepsilon a}\,\frac{Q^m}{(W+\varepsilon a)^m}H_n(a)a^2da, \tag{26,1}$$

$$\eta_n^m=\frac{1}{m}\int\frac{1}{-\varepsilon a}\cdot\frac{Q^m}{(W+\varepsilon a)^m}H_n(a)a^4da, \tag{26,2}$$

$$\zeta_n^m=\frac{1}{m}\int\frac{1}{-\varepsilon a}\,\frac{Q^m}{(W+\varepsilon a)^m}H_n(a)da, \tag{26,3}$$

$$\theta_n^m=\frac{1}{m}\int\frac{1}{-\varepsilon a}\,\frac{Q^m}{(W+\varepsilon a)^m}H_n(a)a^6da, \tag{26,4}$$

$$\Phi_n^m=\frac{1}{m}\int\frac{1}{-\varepsilon a}\,\frac{Q^m}{(W+\varepsilon a)^m}H_n(a)\frac{da}{a^2}, \tag{26,5}$$

$$Q=(W^2-\mu_0^2c^2-a^2)/2, \tag{26,6}$$

$$H_n=1/n\cdot 2ap_e((p_e-a)^2+\lambda'^2)^n. \tag{26,7}$$

(26,1) ~ (26,5) are easily shown to be reduced to the following two types of integrals.

$$J_n^m=\int_{-\sqrt{W^2-\mu_0^2c^2}}^{\sqrt{W^2-\mu_0^2c^2}} u^m/[(p_e-u)^2+\lambda'^2]^n\cdot du, \tag{27,1}$$

$$P_n^m=\int_{-\sqrt{W^2-\mu_0^2c^2}}^{\sqrt{W^2-\mu_0^2c^2}} \varepsilon/(W+\varepsilon u)^m[(p_e-u)^2+\lambda'^2]^n\cdot du. \tag{27,2}$$

Namely, it follows

$$\begin{aligned}
\xi_n^1&=(J_n^1+\mu_0^2c^2P_n^1)/4np_e,\\
\xi_n^2&=(2WJ_n^1+4W\mu_0^2c^2P_n^1-\mu_0^4c^4P_n^2)/16np_e,\\
\xi_n^3&=\{J_n^3+3(W^2+\mu_0^2c^2)J_n^1+3\mu_0^2c^2(4W^2+\mu_0^2c^2)P_n^1-6W\mu_0^4c^4P_n^2\\
&\qquad+\mu_0^6c^6P_n^3\}/48np_e,
\end{aligned} \tag{28,1}$$

$$\begin{aligned}
\eta_n^1&=(J_n^3+\mu_0^2c^2J_n^1+W^2\mu_0^2c^2\cdot P_n^1)/4np_e,\\
\eta_n^2&=\{2WJ_n^3+4W\mu_0^2c^2J_n^1+2W\mu_0^2c^2(2W^2+\mu_0^2c^2)P_n^1-W^2\mu_0^4c^4P_n^2\}/16np_e,\\
\eta_n^3&=\{(J_n^5+3(W^2+\mu_0^2c^2)J_n^3+3\mu_0^2c^2(4W^2+\mu_0^2c^2)J_n^1+\mu_0^2c^2(12W^4\\
&\quad+15W^2\mu_0^2c^2+\mu_0^4c^4)P_n^1-2W\mu_0^4c^4(3W^2+\mu_0^2c^2)P_n^2+W^2\mu_0^6c^6P_n^3\}/48np_e,
\end{aligned} \tag{28,2}$$

$$\begin{aligned}
\zeta_n^1&=\{(W^2-\mu_0^2c^2)/W^2\cdot J_n^{-1}+\mu_0^2c^2/W^2\cdot P_n^1\}/4np_e,\\
\zeta_n^2&=\{2(W^2-\mu_0^2c^2)^2/W^3\cdot J_n^{-1}-2((W^2-\mu_0^2c^2)^2-W^4)/W^3\cdot P_n^1\\
&\qquad-\mu_0^4c^4/W^2\cdot P_n^2\}/16np_e,\\
\zeta_n^3&=\{J_n^1+3(W^2-\mu_0^2c^2)^3/W^4\cdot J_n^{-1}+3\mu_0^2c^2(4W^4-3W^2\mu_0^2c^2+\mu_0^4c^4)\\
&\quad\cdot 1/W^4\cdot P_n^1-2\mu_0^4c^4(3W^2-\mu_0^2c^2)/W^3\cdot P_n^2+\mu_0^6c^6/W^2\cdot P_n^3\}/48np_e,
\end{aligned} \tag{28,3}$$

$$\begin{aligned}
\Phi_n^1&=\{(W^2-\mu_0^2c^2)/W^2\cdot J_n^{-3}-\mu_0^2c^2/W^4\cdot J_n^{-1}+\mu_0^2c^2/W^4\cdot P_n^1\}/4np_e,\\
\Phi_n^2&=\{(-2\mu_0^2c^2(2W^2-3\mu_0^2c^2)/W^3\cdot J_n^{-1}-4\mu_0^2c^2(W^2-\mu_0^2c^2)/W^5\cdot J_n^{-3}\\
&\quad+(W^2-\mu_0^2c^2)/W^3\cdot J_n^{-5}+2\mu_0^2c^2/W^7\cdot P_n^1-\mu_0^4c^4/W^6\cdot P_n^2\}/16np_e,\\
\Phi_n^3&=\{-(W^2-\mu_0^2c^2)(11W^2-2\mu_0^2c^2)/W^6\cdot J_n^{-1}+(W^2-\mu_0^2c^2)^3/W^4\cdot J_n^{-3}\\
&\quad+(W^6+(W^2-\mu_0^2c^2)\cdot(11W^2-2\mu_0^2c^2))/W^6\cdot P_n^1-(2W^6-(19W^2\\
&\quad-4\mu_0^2c^2)(W^2-\mu_0^2c^2))/W^5\cdot P_n^2+\mu_0^6c^6/W^8\cdot P_n^3\}/48np_e,
\end{aligned} \tag{28,4}$$

$$\Theta_n^1=(J_n^5+\mu_0^2c^2J_n^3+W^2\mu_0^2c^2J_n^1+W^4\mu_0^2c^2P_n^1)/4np_e. \tag{28,5}$$

Furthermore, J_n^m and P_n^m can be reduced, by the recurrence formula (see Appendix), to

$$P_1^0=\frac{\varepsilon}{\lambda'}\tan^{-1}\frac{2\lambda'\sqrt{W^2-\mu_0^2c^2}}{\lambda'^2-(W^2-\mu_0^2c^2)+p_e^2}. \tag{29}$$

On expressing the energies and momenta involved in f of (21) by the units of mc^2 and mc respectively, we find, for the required transition probability,

$$P=\frac{g_i^2}{\hbar mc^2}\cdot\left(\frac{mc}{\hbar}\right)^6\frac{1}{36\pi^4}\lambda'^5\bar{f}_i\,d\bar{E}_e, \tag{30}$$

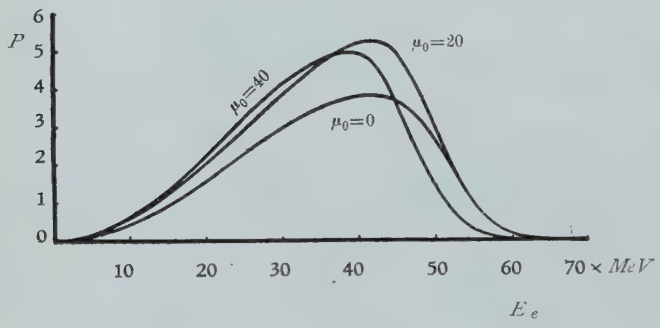
where the dimensionless factor $\bar{f}_i$ has the similar form to that of f_i, except for the replacement of E_e by $\bar{E}_e=E_e/mc^2$ and m=electron mass.

§ 4. Energy spectrum of decay electrons

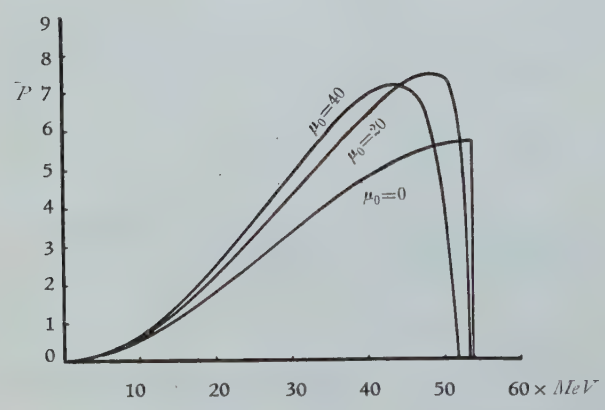
In order to obtain the energy spectra of electrons from μ^- decay, we have numerically evaluated (30) for several values of the mass of neutral particle assumed to be $\mu_0=0$, $20m$, $40m$ and for several forms of coupling in which $Z=26$ (Fe) and $\mu=210m$ have been adopted. The results are described on the left hand side of Fig. $1\sim5$, while, on the right hand side of it, the results of Tiomno and Wheeler, valid for positron from μ^+ decay, are reproduced, for comparison, corresponding to the same values of the various kinds of quantities involved. The units of the ordinates in the figures are $1/36\pi^4\cdot(m/\hbar)^6 g_i^2/mc^2\hbar\cdot(\bar{\mu}\alpha Z)^5$ $(\bar{\mu}=\mu/m=210)$ and those of the abscissa $E_e=E_e/mc^2$. In Fig. 6 the corresponding energy spectra for $\mu=200m$ and $\mu_0=20m$ have been described in order to give some indications regarding the effect of the mass value of μ^- meson upon the spectra.

It will be clearly seen that the electron energy spectra have the enhanced tailing part of relatively small number of electrons near the upper end in comparison with the positron spectra with a relatively large number of positrons near the sharp cutoff. The mentioned difference between both energy spectra could perhaps be observed experimentally by making use of the large intensity of artificially produced mesons in the laboratory if the relatively

Fig 1.

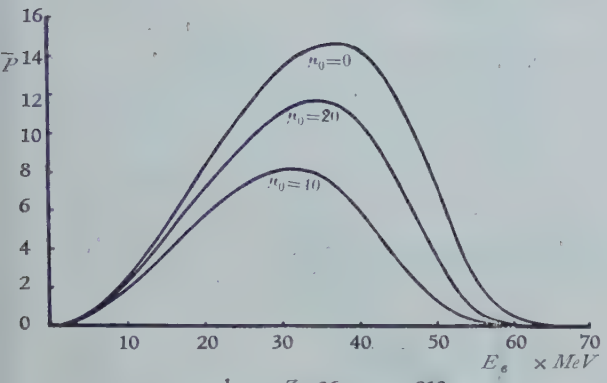


μ^- decay, $Z=26$
$\mu=210m$,
(Scalar coupling)

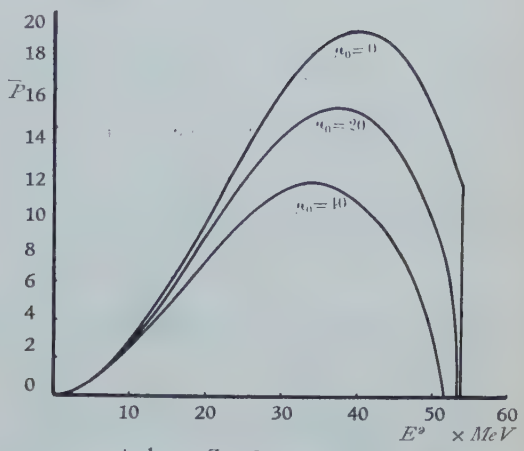


μ^+ decay, $Z=26$
$\mu=210m$,
(Scalar coupling)

Fig. 2.

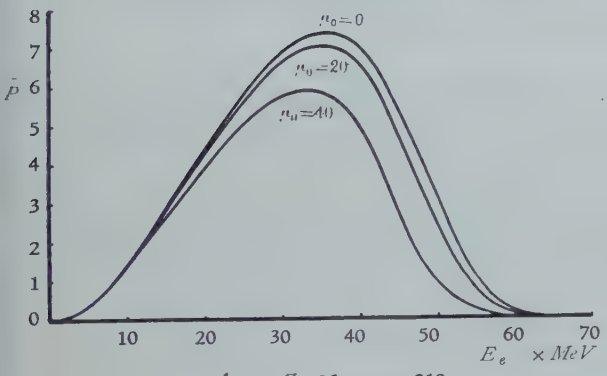


μ^- decay, $Z=26$ $\mu=210$m,
(Vector coupling)

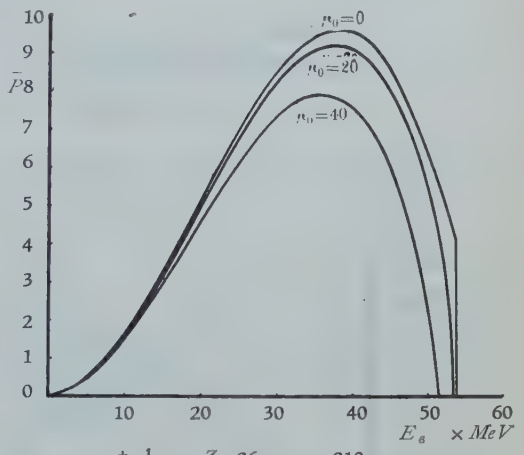


μ^+ decay, $Z=26$ $\mu=210$m,
(Vector couling)

Fig. 3.

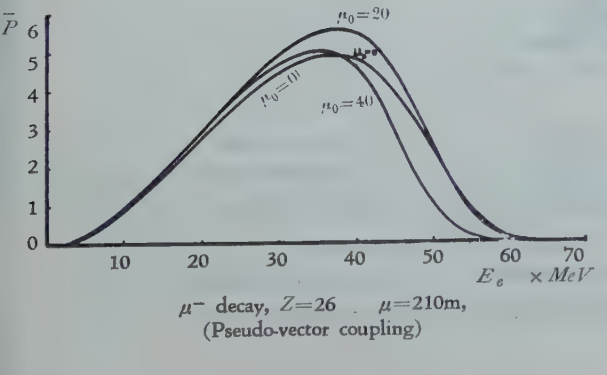


μ^- decay, $Z=26$ $\mu=210$m,
(Tensor coupling)

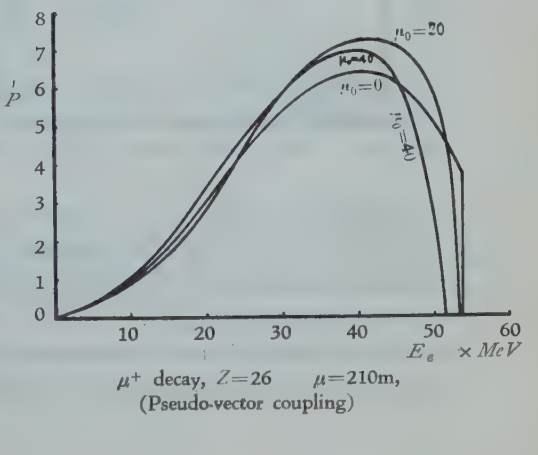


μ^+ decay, $Z=26$ $\mu=210$m,
(Tensor coupling)

Fig. 4.

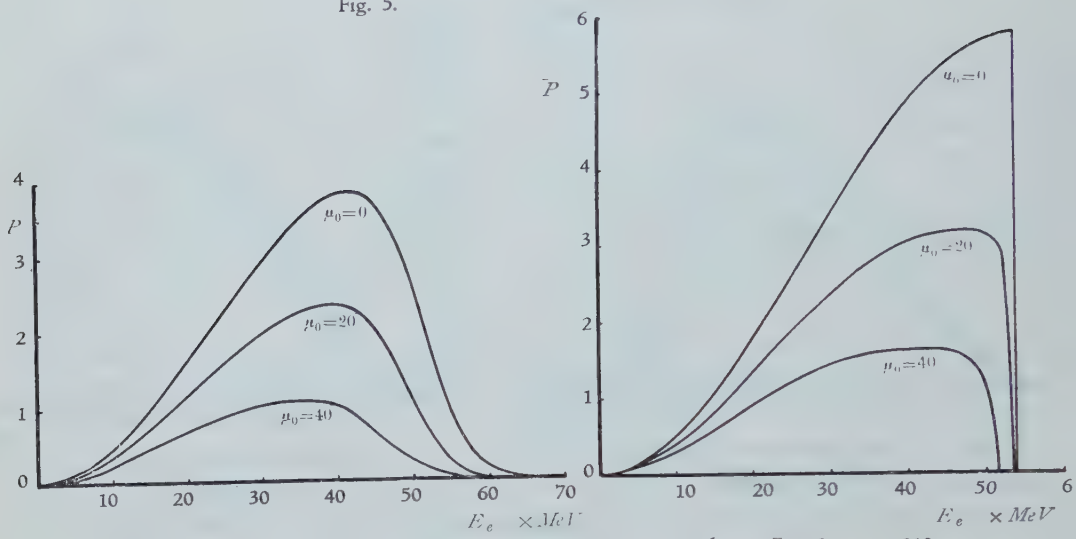


μ^- decay, $Z=26$ $\mu=210$m,
(Pseudo-vector coupling)



μ^+ decay, $Z=26$ $\mu=210$m,
(Pseudo-vector coupling)

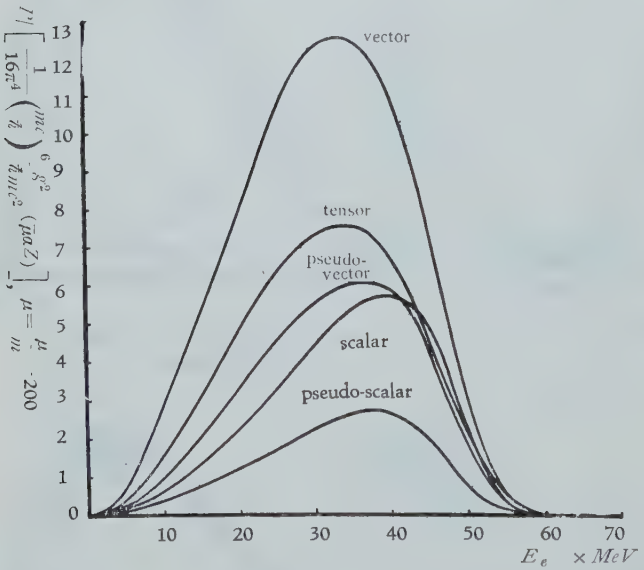
Fig. 5.



μ^- decay, $Z=26$ $\mu=210$m,
(Pseudo-scalar coupling)

μ^+ decay, $Z=26$ $\mu=210$m
(Pseudo-scalar coupling)

Fig. 6



μ^- decay, $Z=26$
$\mu=200$m, $\mu_0=20$m

light element were used as a μ^- meson absorber to avoid the induced decay of μ^- meson by the nearby nucleus. The influences of the mass of a μ_0 particle upon the energy spectra are observed in the figures, being different for the different couplings. It will be extremely desirable, through the accurate measurements of $e^{\pm}$ energy spectra, to decide whether the μ_0 particle is really a neutrino or another neutral particle still unknown, since we, at present, have no information about the neutral counterpart to the $\mu^{\pm}$ meson, correspond-

ing to a neutral π meson (π^0) with respect to the $\pi^{\pm}$ meson.

§ 5. Life time of negative μ meson

The theoretical values of the spontaneous decay life times (τ_n and τ_p) of negative and positive μ meson have been obtained, for a given set of masses and any given form of couplings, by evaluating graphically the area under the curves shown in the diagrams. The values of τ_n/τ_p thus obtained do not depend upon the value of the coupling constants g, the results of which are described in the accompanying table.

Table I

	$\mu_0=40$m			$\mu_0=20$m			$\mu_0=0$		
	τ_n/τ_p	τ_n (10^{-6}sec)	τ_- (10^{-6}sec)	τ_n/τ_p	τ_n (10^{-6}sec)	τ_- (10^{-6}sec)	τ_n/τ_p	τ_n (10^{-6}sec)	τ^- (10^{-6}sec)
Scalar	1.3_5	3.0_0	0.19_8	1.2_9	2.8_6	0.18_9	1.3_4	2.9_7	0.19_6
Pseudo-scalar	1.5_9	3.5_3	0.23_3	1.3_7	3.0_4	0.20_1	1.3_4	2.9_7	0.19_6
Vector	1.4_6	3.2_4	0.21_4	1.3_4	2.9_7	0.19_6	1.3_6	3.0_2	0.19_9
Pseudo-vector	1.4_1	3.1_3	0.20_6	1.2_8	2.8_4	0.18_7	1.3_6	3.0_2	0.19_9
Tensor	1.3_9	3.0_9	0.20_4	1.3_3	2.9_5	0.19_5	1.3_3	2.9_5	0.19_5

$\tau_p=2.22\pm0.02\mu$ sec (Bell-Hincks), $Z_{eff}=19.40(Fe)$, $Z_0=10$.

The total decay life time (τ_-) of a negative μ meson, allowing for both spontaneous and induced decays, is given by the expression[12] of Wheeler

$$\tau_-=\tau_n/(1+(Z_{eff}/Z_0)^4), \qquad (31)$$

where Z_0 represents the atomic number of that idealized nucleus which is able to compete for the induced decay of μ^- meson on equal terms with the process of spontaneous decay, and becomes of about $Z_0=10$. Z_{eff} denotes the effective nuclear charge evaluated numerically by Wheeler[12] and takes the values of 19.40 (Fe), 7.56 (O), 5.78 (C) and 3.925 (Be) respectively.

Since the appreciable decay processes of a positive μ meson are not conceivable beside the spontaneous one,† we have

$$\tau_+=\tau_p. \qquad (32)$$

The recent measurement of Bell and Hincks†† has given for the life time of the μ^+ meson to become of $(2.22\pm0.02)\cdot10^{-6}$ sec[13], which value has been used to obtain τ_n from the theoretical values of τ_n/τ_p in the table. Finally the values of τ_- in Table I have been obtained by the use of (31).

† The possible modes of decay processes, different from the spontaneous one, of μ^+ meson in matter have been discussed theoretically by Muto and Sebe, according to which the cross sections of all possible decay processes become negligibly small in comparison with that of a spontaneous decay. The results of the discussion will shortly appear in the later issue of the journal.

†† The previous values of τ_p are $2.15\pm0.07\mu$ sec (Nerson & Rossi), $2.11\pm0.10\mu$ sec (Ticho), 2.33 ± 0.15 μ sec (Conversi & Piccioni) and 2.09 ± 0.3 μ sec (Alvares).

As seen from Table I, the life times of the spontaneous decay process of μ^- meson become certainly larger compared with that of μ^+ meson for iron, the differences between both life times being actually outside of the experimental errors. Since, however, the atomic number of iron is sufficiently large so that no μ^-.spontaneous decay is recorded experimentally, it will be hopeless to measure τ_n directly for iron. For the direct measurements of τ_n and electron energy spectra, therefore, it is required to adopt a suitable absorber of lighter elements, for example, Be and B.

For the relatively heavy elements, i.e., iron, it is highly desirable for the measurement of τ_-, expected theoretically to be different from τ_p, to be carried out in order to clarify the detailed behaviours of both μ meson decay process in matter. Finally it should be remarked that the careful examination of (30) reveals that the spontaneous life time of negative μ meson (τ_n) is roughly proportional to Z^{-5}.

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Appendix

(Recurrence formula of P_n^m and J_n^m)

$$P_2^0=\varepsilon\{(M_1^+ + M_1^-)/2\lambda'^2 + P/2\lambda'^2\},$$

$$P_3^0=\varepsilon\{(M_3^+ + M_3^-)/4\lambda'^2 + 3(M_1^+ + M_1^-)/8\lambda'^4 + 3P/8\lambda'^4\},$$

$$P_1^1=1/2(l^2+\lambda'^2)\cdot\log M_0^-/M_0^+ + \varepsilon/(l^2+\lambda'^2)\cdot(R'+lP),$$

$$P_2^1=1/2(l^2+\lambda'^2)\cdot\{(M_0^- - M_0^+) + \varepsilon l(M_1^+ + M_1^-)/\lambda'^2 + \varepsilon l(l^2+3\lambda'^2)P/\lambda'^2(l^2+\lambda'^2) + 2\varepsilon R^1/(l^2+\lambda'^2) + 1/(l^2+\lambda'^2)\cdot\log M_0^-/M_0^+\},$$

$$P_3^1=\{M_2^- - M_2^+ + 4lP_3^0 + 3P_2^1\}/4(l^2+\lambda'^2),$$

$$P_3^2=\{-[W(M_2^- - M_2^+) - \varepsilon\sqrt{W^2-\mu_0^2c^2}\cdot(M_2^+ + M_2^-)]/\mu_0^2c^2 + 6lP_3^1 - 5P_3^0\}/(l^2+\lambda'^2),$$

$$P_2^2=\{-[W(M_0^- - M_0^+) - \varepsilon\sqrt{W^2-\mu_0^2c^2}\cdot(M_0^+ + M_0^-)]/\mu_0^2c^2 + 4lP_2^1 - 3P_2^0\}/(l^2+\lambda'^2),$$

$$P_3^3=\{-[(2W^2-\mu_0^2c^2)(M_2^- - M_2^+) - 2\varepsilon W\sqrt{W^2-\mu_0^2c^2}(M_2^+ + M_2^-)]/2\mu_0^4c^4 + 4lP_3^2 - 3P_3^1\}/(l^2+\lambda'^2),$$

$$P_2^3=\{-[(2W^2-\mu_0^2c^2)(M_0^- - M_0^+) - 2\varepsilon W\sqrt{W^2-\mu_0^2c^2}(M_0^+ + M_0^-)]/2\mu_0^4c^4 + 3lP_2^2 - 2P_2^1\}/(l^2+\lambda'^2),$$

$$J_2^1=p_e|P_2^0| - (M_0^- - M_0^+)/2,$$

$$J_3^1=p_e|P_3^0| - (M_2^- - M_2^+)/4,$$

$$J_3^3=-(W^2-\mu_0^2c^2)(M_2^- - M_2^+)/2 + (p_e^2+\lambda'^2)J_3^1,$$

$$M_0^\pm=1/[(\sqrt{W^2-\mu_0^2c^2}\pm p_e)^2+\lambda'^2],$$

$$M_1^\pm=(\sqrt{W^2-\mu_0^2c^2}\pm p_e)/((\sqrt{W^2-\mu_0^2c^2}\pm p_e)^2+\lambda'^2),$$

$$M_2^{\pm}=(M_0^{\pm})^2, M_3^{\pm}=(\sqrt{W^2-\mu_0^2c^2}\pm p_e)\cdot M_2^{\pm},$$

$$P=1/\lambda'\cdot\tan^{-1}\{2\lambda'\sqrt{W^2-\mu_0^2c^2}/(\lambda'^2+p_e^2-W^2+\mu_0^2c^2)\},$$

$$R'=\log\{(W+\sqrt{W^2-\mu_0^2c^2})/(W-\sqrt{W^2-\mu_0^2c^2})\},$$

$l=W\pm p_e$ corresponding to $\varepsilon=1$ and -1 respectively.

References

1) Fermi, Teller and Weisskopf, Phys. Rev. **72** (1947), 314.
Fermi and Teller, Phys. Rev. **72** (1947), 399.
Hubby, Phil. Mag. **48** (1949), 685.
Wheeler, Rev. Mod. Phys. **21** (1949), 133.
2) Wheeler, loc. cit.; Tiomno and Wheeler, Rev. Mod. Phys. **21** (1949), 153; Chang, Rev. Mod. Phys. **21** (1949), 166.
3) Wheeler and Tiomno, loc. cit.
4) Tiomno and Wheeler, Rev. Mod. Phys. **21** (1949), 144.
5) Steinberger, Phys. Rev. **75** (1949), 1136.
6) Leighton, Anderson and Seriff, Phys. Rev. **75** (1949), 1432.
7) Sagane et al., Phys. Rev. **82** (1951), 557.
8) Porter and Primakoff, Phys. Rev. **83** (1951), 849.
9) Tiomno and Wheeler, loc. cit.
10) Heitler, *The Quantum Theory of Radiation* (1944).
11) Porter and Primakoff adopted non-relativistic wave function for the bound μ meson.
12) Wheeler, loc. cit.
13) Bell and Hincks, Phys. Rev. **84** (1951), 1243.
14) Nerson and Rossi, Phys. Rev. **64** (1943), 199.
15) Ticho, Phys. Rev. **74** (1948), 1337.
16) Conversi and Piccioni, Phys. Rev. **70** (1946), 859.
17) Alvares, Phys. Rev. **77** (1950), 752.

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Note on the Non-Local Interaction*

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In order to construct the singularity free classical electrodynamics, Bopp[1] proposed to generalize the field equation and Peierls-McManus[2] attempted the extension of the interaction. In this paper, we investigate first the interrelations between these two theories from the quantum-theoretical point of view. Then two special types of the non-local interaction between electromagnetic field and an electron are proposed, with which the problem of the self-charge as well as the electron self-energy can be treated satisfactorily.

§ 1. Introduction

To avoid the divergence difficulties of the quantum field theory, various investigations have been made by modifying or generalizing the conventional formalism. Most of them put their hands to this problem from a classical point of view. Among them the work of Bopp[1] should be noted. This author studied especially the following generalization of the electromagnetic theory:

$$\Box(\Box-\mu^2)A_\mu(x)=-\frac{1}{c}j_\mu(x)$$

and showed that it leads to a classical theory which is singularity free and goes over into the conventional theory for distances $\gg\mu^{-1}$. After him many investigations, containing the quantum-theoretical ones, have been done along this line from various points of view. In particular, Pais-Uhlenbeck's investigation[3] was most exhaustive, and by this investigation, defects of the Bopp-type theory as well as its merits were clarified. On the other hand, Peierls-McManus[2] investigated this problem along another line. Namely, by taking

$$\frac{1}{c}\iint j_\mu(x)\eta(x,x')A_\mu(x')(d^4x)(d^4x'),$$

they assumed the interaction between electromagnetic and electron fields to be non-local, and then examined the electromagnetic theory of local fields within the frame of classical mechanics.

These two theories start from different standpoints and it seems that, at first sight, they have no mutual connection with each other. But, as will be shown in the following

* This note is the revision of the report read before the meeting of the Physical Society held in January 1950, at Osaka University.

paragraphs, Bopp's formalism of generalized field and Peierls-McManus' formalism of non-local interaction (to be designated hereafter as FGF and FNI respectively) have close connections. Although the investigation of the interrelation between these two theories is the chief purpose of this paper, the study of FNI will be done quantum-theoretically in various types of $\eta(x, x')$. After these investigations, we shall propose two special types of FNI, with which the problem of the self-charge as well as that of the electron self-energy can be dealt satisfactorily.

As the recent investigations show,[4] in some sorts of interactions (e.g. the direct interaction between four spinor particles) we are obliged to introduce infinite number of counter interactions having successively higher derivatives of field variables when we attempt to remove the divergences by means of the renormalization method; the renormalized interactions thus obtained are non-local. Consequently, the present work may also have a rôle of the preparation for future investigations of such non-localized interactions as in the renormalization procedure.

§ 2. Formalism of the non-local interaction (FNI)

In FNI, we investigate the interacting system of electrons and electromagnetic field by taking the following Lagrangian:

$$\bar{L}=-\frac{1}{2}\int(\partial_\nu A_\mu(x))^2\,(d^4x)-\frac{\hbar c}{2}\int\{\bar{\psi}(x)\,(\gamma_\mu\partial_\mu+\mu_0)\psi(x)+\text{charge conj.}\}(d^4x)$$
$$+\frac{1}{c}\iint j_\mu(x)\,\eta(x,x')\,A_\mu(x')\,(d^4x)\,(d^4x'). \tag{1}$$

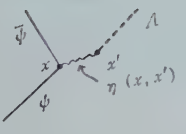

Fig. 1

The structure of this interaction is graphically represented in Fig. 1. The Lagrangian is invariant under the following gauge transformation:

$$\begin{cases}A_\mu(x)\to A_\mu(x)-\partial_\mu\Lambda(x), & \Box\Lambda(x)=0,\\ \psi(x)\to\psi(x)\,\exp\left\{-\dfrac{ie}{\hbar c}\displaystyle\int\eta(x,x')\,\Lambda(x')\,(d^4x')\right\}.\end{cases} \tag{2}$$

The equation for the electromagnetic field derived from the Lagrangian (1) is

$$\Box A_\mu(x)=-\frac{1}{c}\int\eta(x,x')j_\mu(x')\,(d^4x'), \tag{3}$$

and the general solution of eq. (3) has the form

$$A_\mu(x)=A_\mu{}^\circ(x)+\frac{1}{c}\int\bar{D}(x-x'')\,(d^4x'')\int\eta(x'',x')\,j_\mu(x')\,(d^4x'), \tag{4}$$

where A_μ^0 is the general solution of the homogeneous equation associated with (3). If η is the Lorentz invariant scalar function and representable as

$$\eta(x'',x')=\frac{1}{(2\pi)^4}\int(d^4k)F(k^2)e^{ik(x''-x')}, \tag{5}$$

we can write

$$\int \bar{D}(x-x'')(d^4x'')\,\eta(x'',x') = \frac{1}{(2\pi)^4} P\int (d^4k)\cdot F(k^2)/k^2 \cdot e^{ik(x-x')}$$

$$\equiv \frac{1}{(2\pi)^4} P\int (d^4k)\, G(k^2)\, e^{ik(x-x')} \equiv \bar{g}(x-x'), \tag{6}$$

and accordingly

$$\Box \bar{g}(x-x') = -\eta(x,x'). \tag{7}$$

Besides the requirement (5), we must impose upon η the normalization condition:

$$\int \eta(x)(d^4x) = 1, \quad \text{accordingly} \quad F(0) = 1. \tag{8}$$

In FGF, the same function $\bar{g}(x)$ as (6) also appears in $A_\mu(x)$ as the propagation function which represents the attached potential. Consequently, our investigations of interrelations between FNI and FGF will be made mainly by comparing the properties of $\bar{g}$-function.

As is seen in the above representation, $\eta(x)$ changes the propagation function $\bar{D}(x)$ into $\bar{g}(x)$, while, defining

$$\int \eta(x'',x')\, j_\mu(x')(d^4x') \equiv \bar{j}_\mu(x''), \tag{9}$$

it can also be interpreted as modifying the charge-current density $j_\mu(x')$ ($\bar{j}_\mu(x'')$ is, so to speak, the effective extended charge-current density).

The equation for the electron field derived from the Lagrangian (1) is

$$(\gamma_\mu \partial_\mu + \mu_0)\,\psi(x) = (ie/\hbar c)\,\gamma_\mu \psi(x) \int \eta(x,x')\, A_\mu(x')\,(d^4x'), \tag{10}$$

of which the general solution has the form

$$\psi(x) = \psi^\circ(x) - (ie/\hbar c)\int \bar{S}(x-x')\,\gamma_\mu \psi(x')\,\bar{A}_\mu(x')\,(d^4x'), \tag{11}$$

where

$$\bar{A}_\mu(x') = \int \eta(x',x'')\,A_\mu(x'')\,(d^4x'') \tag{11'}$$

and ψ° is the wave function for free electron. Here, one can easily see from the expressions (11) and (11') that the extension function $\eta(x',x'')$ cannot modify the propagation function $\bar{S}(x-x')$ of the electron field contrary to the case of the electromagnetic field represeted by (4) and (6).

The S-matrix in this case can be obtained by the method of Yang-Feldman[5] or of Källén.[6] (Koba[7] has also obtained the generalized S-matrix from the different standpoint.) By using this S-matrix, we can compute the observable quantities for any process. We must, here, call our attension to the fact that the S-matrix does not become the infinitesimal transformation function unless the extension function $\eta(x,x')$ can be represented formally as

$$\eta(x,x') = F(-\Box)\,\delta^4(x,x'). \tag{12}$$

In the case that (12) holds, the theory of the non-local interaction is reduced to that of the local interaction which contains higher derivatives of field variables. And, in order to be able to write as (12), $F(k_\mu^2)$ must be analytic within the interval $-\infty < k_\mu^2 < +\infty$; namely $F(k_\mu^2)$ must be such a function as can be expanded by power series of k_μ^2 and cannot have any pole within the interval $-\infty < k_\mu^2 < +\infty$.

Next, in order to compare with FGF, we shall conveniently take the viewpoint that $\bar{D}(x)$ is replaced by $\bar{g}(x)$, and shall classify $\bar{g}(x)$ into two types: (i) Oscillation type, (ii) Decay type.

(i) *Oscillation type*:

We call such $\bar{g}(x)$ the oscillation type one that has following characteristics: (a) it is regular on the light-cone, (b) $F(k^2)$ has finite or infinite poles and be decomposed into partial fraction. The case of finite poles corresponds to the rational function $F(k^2)$; i.e.

$$\begin{cases} F(k^2)=N(k^2)/M(k^2)=\sum_{j=1}^{n}\xi_j/(k^2+\omega_j^2), \text{ deg. } (N) < \text{deg. } (M), \\ \xi_j=N(-\omega_j^2)/[dM(k^2)/d(k^2)]_{k^2=-\omega_j^2}=N(-\omega_j^2)/M'(-\omega_j^2), \end{cases} \tag{13}$$

where M and N are rational function of k^2 and $-\omega_j^2$'s are the roots of $M(k^2)=0$, namely

$$M(k^2)=\prod_{i=1}^{n}(1+k^2/\omega_i^2).$$

Besides the poles of $F(k^2)$ given by (13) $G(k^2)$ has another pole $1/k^2$, because $G(k^2)$ is connected with $F(k^2)$ by the definition (6). Therefore, in order to obtain the regularized $\bar{g}(x)$ on the light-cone the number of poles of $F(k^2)$ must be odd. The case of infinite poles corresponds to the transcendental function $F(k^2)$ which satisfies the condition (8).

In both cases, assuming that $f(k^2)$ has no multiple root, the characteristics of this type is represented by the following expression of $F(k^2)$ (or $G(k^2)$):

$$\begin{cases} F(k^2)=1/f(k^2), \quad f(k^2)=\prod_{i=1}(1+k^2/\omega_i^2), \\ G(k^2)=1/k^2f(k^2)=\sum_{j=0}\xi_j/(k^2+\omega_j^2), \end{cases} \tag{14}$$

where

$$\xi_0=1, \quad \omega_0=0; \quad \xi_i=-1/\omega_i^2 f'(-\omega_i^2), \qquad (i=1, 2, \cdots),$$

and

$$\sum_{j=0}\xi_j\omega_j^{2n}=0, \qquad (n=0, 1, 2, \cdots). \tag{15}$$

Then, as each term of the expansion of $G(k^2)$ corresponds to the usual $\bar{\Delta}(x, \omega_j)$-function in the coordinate space, $\bar{g}(x)$ consists of the superposition of $\bar{\Delta}(x, \omega_j)$-functions which have singularities on the light-cone. However, $\bar{g}$ itself is regular on the light-cone, because the singularities of $\bar{\Delta}$'s are canceled each other by means of the condition (15). Moreover, $\bar{g}$ vanishes in the space-like region in accordance with the properties of $\bar{\Delta}$-function and can be decomposed into

$$\bar{g}(x)=\frac{1}{2}\{g_{\mathrm{ret}}(x)+g_{\mathrm{adv}}(x)\}, \tag{16}$$

which assures existence of the law of causality.

When $G(k^2)$ is given by (14), the charge distribution and the static potential of the electron located at the origin are given respectively by

$$e\rho(r)=-\frac{e}{4\pi}[\sum_{i=1}\xi_i\omega_i^2\exp(-\omega_i r)]/r, \tag{17}$$

and

$$e\phi(r)=e[1+\sum_{i=1}\xi_i\exp(-\omega_i r)]/r. \tag{18}$$

Both these two quantities are singularity free at the origin owing to (15). And (17) shows that the charge distribution of the electron has the three dimensional extension notwithstanding the extension function $\eta(x)$ vanishes in the space-like region.

We can avoid, in the oscillation type, the difficulty of the "energy-indefiniteness" which appears in FGF, because the free boson field contains only photon. There appears, however, a new difficulty[5] that the electron gets energy while emitting photons and this corresponds to the energy-indefiniteness of FGF. If we interprete, in accordance with the fact represented in (17), that the domain where $\bar{g}(x)$ does not vanish, excluding the light-cone, corresponds to the extension of the electron, the electron has the infinite extension.

$\bar{g}$ of this type gives the same convergent effect on the self-energy of the electron as the corresponding type of FGF (formalism of the formal mixture of various mesons with the photon) owing to the automatic regularization condition (15) of Pauli-Villars[9]. Indeed, the self-energy integral in the S-matrix, which is not the infinitesimal transformation function, is given by (see Fig. 2)

$$\frac{e^2}{\hbar c}\int(d^4p)\,\bar{\psi}(p)\int(d^4k)\left[\gamma_\mu\frac{\{i\gamma(p-k)-\mu_0\}}{(p-k)^2+\mu_0^2}\gamma_\mu\frac{F^2(k^2)}{k^2}\right]\psi(p).$$

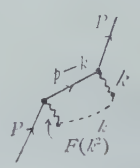

Fig. 2

Here we must use the partial fraction expansion and the condition (15) to the factor $F^2(k^2)/k^2$ without factorizing each $F(k^2)$. This type is powerless, however, to treat the problem of the vacuum polarization, because the propagation function $\bar{S}(x)$ cannot be modified by $\eta(x)$.

(ii) *Decay type*:

We call such $\bar{g}(x)$ the decay type one that is regular on the light-cone (condition (a)) and approaches rapidly to zero according as $|x_\mu^2|$ becomes larger and larger (condition (b)). The condition (a) secures the finiteness of the electron self-energy. In order to satisfy the requirement (b), at least $G(k^2)$ cannot have any pole.

By means of the condition (b), we can avoid the difficulty mentioned as for the oscillation type and the extension of the electron does become finite in this type. Of cource, the difficulty of energy-indefiniteness does not occur.

$\bar{g}$ of this type does not vanish in general in the space-like region and cannot be separated into g_{ret} and g_{adv}. Consequently the law of causality is broken in the region where $\bar{g}$ survives except on the light-cone.

The contents of the theory of this type are equivalent to that of FGF[10] having the following equation for the electromagnetic field

$$\begin{cases} \Box f(\Box) A_\mu(x) = -\frac{1}{c} j_\mu(x), \\ \partial_\mu A_\mu(x) = 0, \end{cases} \tag{19}$$

provided that the form of f in (19) is the same as the corresponding one of FNI which is obtained by putting $F(k^2) = 1/f(k^2)$ in (5). Among these equivalent types the following should be noted :

$$F(k^2) = 1/f(-k^2) = \exp(-\lambda^4 k^4). \tag{20}$$

The S-matrix in this type has the infinitesimal transformation character because of (12). The electron self-energy becomes finite so long as the suitable $F(k^2)$ is taken. In this type, however, we need not make use of the partial fraction expansion and the condition (15), as $F(k^2)$ has no pole. As to the problem of the vacuum polarization, this type is powerless in the same way as the oscillation type.

In FGF, the exponential type (20) has been proposed to be the most promising one after the thorough investigations by Pais-Uhlenbeck. In FNI, there exists no superiority or inferiority between the exponential type (in general, the decay type of (ii)) and the other type (the oscillation type of (i)) so far as the problem of convergence is concerned, but physically the decay type seems to be superior to any other one.

§ 3. Formalism of the generalized field (FGF)

In the previous section we discussed the relations between FNI and FGF to some extent, though our discussion was mainly concerned with the former. In this section, we shall investigate the mutual connections between them in more detail.

In FGF, we can take in general the equation of the electromagnetic field interacting with the electron as follows :

$$\begin{cases} \Box f(\Box) A_\mu(x) = -\frac{1}{c} \int \eta(x, x') j_\mu(x') (d^4 x'), \\ \partial_\mu A_\mu(x) = 0. \end{cases} \tag{21}$$

In the following we shall take, however, the point electron by putting $\eta(x, x') = \delta^4(x, x')$ in (21). This restriction is not essential to FGF, but is introduced only for convenience, in order to illustrate clearly the relations between FNI and FGF. The solution of the eq. (21) becomes :

$$\begin{cases} A_\mu(x) = A_\mu^{\circ}(x) + \dfrac{1}{c}\int \bar{g}(x-x')\, j_\mu(x')\,(d^4x'), \\ \bar{g}(x) = \dfrac{1}{(2\pi)^4} P\int (d^4k)\, \dfrac{1}{k^2 f(-k^2)}\, e^{ikx}. \end{cases} \tag{22}$$

Therefore, concerning the propagation problem of radiations from the source, there exist the same circumstances as in FNI. In FGF, however, the most important point lies in the fact that the free electromagnetic field is generally different from the usual Maxwell's one —A_μ° is the general solution of the equation $\Box f(\Box) A_\mu = 0$ – and it consists of the mixture of meson fields of various masses. So that, the free boson field of FGF differs very much from that of FNI.

We can classify FGF into two types (i) and (ii) in accordance with $1/f(-k^2)$ in (22) has poles or no pole, and shall compare them with the corresponding types in FNI.

(i) The case that $1/f(-k^2)$ *has poles*:

The propagation character of radiations from the source in this type is identical with that in oscillation type of FNI. But, there is a wide difference concerning the free boson field. That is, although the free boson field for the oscillation type of FNI is the Maxwell field, the one for this type of FGF deviates largely from the Maxwell field. (We notice here the fact that the difficulty of energy-indefiniteness of this type cannot be avoided even if we take $1/f(-k^2)$ having infinite number of poles—mixture of infinite number of various meson fields containing the negative energy one.)

The S-matrix for this type has the infinitesimal transformation chatacter contrary to that for the oscillation type of FNI.

We shall not go into further discussion on the relations between them, since we can easily see them by comparing the results investigated in (i) of § 2 with the already known facts on this type.

(ii) The case that $1/f(-k^2)$ *has no pole*:

The propagation character of radiations in this type is identical with that in the decay type of FNI. And, as the free boson field satisfies the usual Maxwell equation, the general solution $A_\mu(x)$ of this type is entirely equivalent to that of the decay type of FNI. This equivalency for the boson field holds even if the equations for the electron field in both types differ from each other.

If we retain the usual form for the electron field and start from the Lagrangian desity

$$L(x) = -\frac{1}{2}(\partial_\nu A_\mu(x)) f(\Box)(\partial_\nu A_\mu(x)) - \frac{\hbar c}{2}\{\bar{\psi}(x)(\gamma_\mu\partial_\mu + \mu_0)\psi(x) + \text{charge conj.}\} + \frac{1}{c} j_\mu(x) A_\mu(x), \tag{23}$$

the electron self-energy integral in the S-matrix, which has the infinitesimal transformation character, is given by

$$\frac{e^2}{\hbar c}\int (d^4p)\bar{\psi}(p)\int (d^4k)\left[\gamma_\mu \frac{\{i\gamma(p-k)-\mu_0\}}{(p-k)^2+\mu_0^2}\gamma_\mu \frac{1}{k^2 f(-k^2)}\right]\psi(p),$$

On the other hand, the corresponding integral in the decay type of FNI becomes

$$\frac{e^2}{\hbar c}\int(d^4p)\bar{\psi}(p)\int(d^4k)\left[\gamma_\mu\frac{\{i\gamma(p-k)-\mu_0\}}{(p-k)^2+\mu_0^2}\gamma_\mu\frac{1}{k^2f^2(-k^2)}\right]\psi(p),$$

where $1/f^2(-k^2)=F^2(k^2)$. Notwithstanding the forms of the electromagnetic potential $A_\mu(x)$ .in both types are the same, that of S-matrices differ. Namely, as easily seen from the above two integrals, the propagation function of internal photons in the S-matrices for FGF and FNI are given by $1/k^2f(-k^2)$ and $1/k^2f^2(-k^2)$ respectively in the momentum space.

In the vacuum polarization integral for the type (23) coincides completely with the traditional one. But, in the decay type of FNI, it is given by

$$\left(\frac{e}{\hbar c}\right)^2\int(d^4k)\,A_\mu(k)\,A_\nu(k)F^2(k^2)\int(d^4p)\,S_\rho\left[\frac{\{i\gamma p-\mu_0\}}{p^2+\mu_0^2}\gamma_\mu\frac{\{i\gamma(k-p)-\mu_0\}}{(k-p)^2+\mu_0^2}\gamma_\nu\right].$$

Therefore both types are incompetent as to the problem of the vacuum polarizatien.

As the most generalized form of this case, we can take the following Lagrangian density by assuming that both $1/f(-k^2)$ and $1/h(-k^2)$ have no pole:

$$L(x)=-\frac{1}{2}(\partial_\nu A_\mu(x))f(\Box)(\partial_\nu A_\mu(x))-\frac{\hbar c}{2}\{\bar{\psi}(x)(\gamma_\mu\partial_\mu+\mu_0)h(\Box)\psi(x)$$
$$+\text{charge conj.}\}+\frac{1}{c}j_\mu(x)A_\mu(x). \tag{24}$$

Then we can obtain not only the finite self-energy of the electron but also the finite self-charge. The type of non-local interaction, which has the same effect as this concerning the problem of electron self-energy and of vacuum polarization, will be shown in the next section.

§ 4. Other types of FNI

In the previous two sections, we studied some types of FNI which was closely connected with FGF. In this section, restricting $\eta(x)$ within a scalar function we shall propose the other types of FNI which will be useful for the problem of the vacuum polarization as well as the self-energy of the electron. The characteristics of these types of FNI will be found in that the non-locality of interaction will be taken into account for the electron field.

Starting from the Lagrangian

$$\bar{L}=\bar{L}_m+\bar{L}_f+\bar{L}', \tag{25}$$

where $\bar{L}_m$ and $\bar{L}_f$ are the parts for the conventional electron field and electromagnetic field respectively and $\bar{L}'$ is the interaction part, we can obtain two types (A) and (B) in accordance with the forms of $\bar{L}'$ in (25) as will be seen in what follows.

(A) The type which has the following interaction part:

$$\bar{L}'=ic\iiint\bar{\psi}(x')\eta(x',x)\gamma_\mu A_\mu(x)\eta(x,x'')\psi(x'')(d^4x')(d^4x)(d^4x''). \tag{26}$$

The structure of this interaction is graphically represented in Fig. 3. The field equations derived from (25) and (26) are:

$$\Box A_\mu(x) = -ie\iint \bar{\psi}(x')\eta(x', x)\gamma_\mu\eta(x, x'')\psi(x'')(d^4x')(d^4x''), \qquad (27a)$$

and

$$(\gamma_\mu\partial_\mu + \mu_0)\psi(x) = (ie/\hbar c)\iint \eta(x, x')\gamma_\mu A_\mu(x')\eta(x', x'')\psi(x'')(d^4x')(d^4x''). \qquad (27b)$$

As is seen by comparing Fig. 3 with Fig. 1, the physical significance of the interaction of type (26) may be fond in that the non-locality of interaction is taken into account for material field, while, in Peierls-McManus' theory (Fig. 1) rather the non-locality of photon field was considered.

Next, we shall refer to some characters of the S-matrix for this type of interaction. Namely, we shall observe how the influences of η will be presented in the development of the S-matrix by constructing, for example, two integrals of the electron self-energy and the vacuum polarization. The electron self-energy integral in the S-matrix will be given to the first order as follows (see Fig. 4a):

$$\frac{e^2}{\hbar c}\int (d^4p)F(p)\bar{\psi}(p)\int (d^4k)\left[\gamma_\mu \frac{F^2(p-k)\{i\gamma(p-k)-\mu_0\}}{(p-k)^2+\mu_0^2}\gamma_\mu \frac{1}{k^2}\right]\psi(p)F(p). \qquad (28a)$$

In the problem of the vacuum polarization, we shall have the following integral to the first order (see Fig. 4b):

$$\left(\frac{e}{\hbar c}\right)^2\int (d^4k)A_\mu(k)A_\nu(k)\int (d^4p)\ S_p\left[\frac{F^2(p)\{i\gamma p-\mu_0\}}{p^2+\mu_0^2}\gamma_\mu \frac{F^2(k-p)\{i\gamma(k-p)-\mu_0\}}{(k-p)^2+\mu_0^2}\gamma_\nu\right]. \qquad (28b)$$

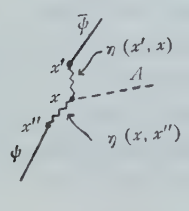

Fig. 3

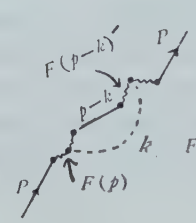

Fig. 4a

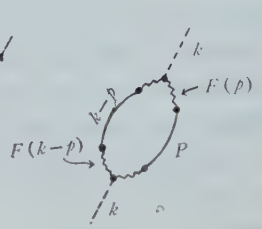

Fig. 4b

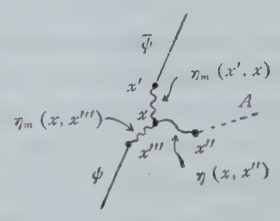

Fig. 5

From these two integrals, we can easily see that η modifies the propagation function of the internal electron field $((i\gamma p-\mu_0)/(p^2+\mu_0^2)$ is modified into $F^2(p)(i\gamma p-\mu_0)/(p^2+\mu_0^2)$ in the momentum space). And the external electron field is also changed from $\psi(p)$ into $\psi(p)F(p)$.

The above two integrals converge so long as the suitable form of $F(p)$ (suitable form of $\eta(x)$) is taken. It seems to us that the decay type η is desirable from the physical point of view.

We can translate the theory of this interaction into the theory of the non-local field, which is formed by a non-local electron and a local electromagnetic field and has the same S-matrix as the former.

(B) We may take another type of the non-local interaction by giving $\bar{L}'$ in (25) as follows:

$$\bar{L}'=ie\iiiint\bar{\psi}(x')\eta_m(x',x)\gamma_\mu\eta_m(x,x''')\psi(x''')\eta_f(x,x'')A_\mu(x'')(d^4x)(d^4x')\cdot\cdot(d^4x'')(d^4x'''). \tag{29}$$

The structure of this interaction is graphically represented in Fig. 5. The field equations derived from (25) and (29) are:

$$\Box A_\mu(x)=-ie\iiint\eta_f(x,x'')\bar{\psi}(x')\eta_m(x',x'')\gamma_\mu\eta_m(x'',x''')\cdot\cdot\psi(x''')(d^4x')(d^4x'')(d^4x'''), \tag{30a}$$

and

$$(\gamma_\mu\partial_\mu+\mu_0)\psi(x)=(ie/\hbar c)\iiint\eta_m(x,x')\gamma_\mu\eta_m(x',x''')\psi(x''')\cdot\cdot\eta_f(x',x'')A_\mu(x'')(d^4x')(d^4x'')(d^4x'''), \tag{30b}$$

where η_m for the electron field need not be equal to η_f for the electromagnetic field.

The electron self-energy integral and the vacuum polarization integral in the S-matrix will be given to the first order by

$$\frac{e^2}{\hbar c}\int(d^4p)F_m(p)\bar{\psi}(p)\int(d^4k)\left[\gamma_\mu\frac{F_m^2(p-k)\{i\gamma(p-k)-\mu_0\}}{(p-k)^2+\mu_0^2}\gamma_\mu\frac{F_f^2(k)}{k^2}\right]\psi(p)F_m(p), \tag{31a}$$

and

$$\left(\frac{e}{\hbar c}\right)^2\int(d^4k)A_\mu(k)A_\nu(k)F_f^2(k)\int(d^4p)\,S_p\cdot\cdot\left[\frac{F_m^2(p)\{i\gamma p-\mu_0\}}{p^2+\mu_0^2}\gamma_\mu\frac{F_m^2(k-p)\{i\gamma(k-p)-\mu_0\}}{(k-p)^2+\mu_0^2}\gamma_\nu\right], \tag{31b}$$

respectively, where $F_m(p)$ and $F_f(k)$ are Fourier transforms of $\eta_m(x)$ and $\eta_f(x)$. From these two integrals, we can easily see that η_m and η_f modify the propagation function of the internal electron field and the internal photon field respectively. Namely, $(i\gamma p-\mu_0)/(p^2+\mu_0^2)$ for the electron field is changed into $F_m^2(p)(i\gamma p-\mu_0)/(p^2+\mu_0^2)$ and $1/k^2$ for the photon field is changed into $F_f^2(k)/k^2$. Moreover, the external electron field and the photon field are also modified into $\psi(p)F_m(p)$ and $A_\mu(k)F_f(k)$ respectively. The above two integrals, (31a) and (31b), will converge when the suitable forms of $F_m(p)$ and $F_f(k)$ (i.e. $\eta_m(x)$ and $\eta_f(x)$) are taken.

We can translate the theory of this interaction into the theory of the non-local field, which is formed by a non-local electron and a non-local electromagnetic field. Also, this type has some connections with the type (24) when in the former a decay type of η_m and of η_f are taken.

It must be noted that, in both cases (A) and (B), the effects of convergence factor η occur also in the integrals concerning real processes in the S-matrix. This and some other problems concerning the non-local theory stated in this section are left in future.

We wish to express our sincere thanks to Prof. Y. Mimura and Prof. K. Sakuma for their kind interest in this work, and also to Mr. T. Yamauchi (Kyûshû University, Fukuoka) for his valuable advices for the work of § 2.

References

1) F. Bopp, Ann. d. Physik **38** (1940), 345.
F. Bopp et al., Ann. d. Physik **42** (1943), 572; ZS. f. Naturforshg. **1** (1946), 237; ZS. f. Phys. **125** (1949), 615.
(We go through the list of the theories which are equivalent to the Bopp's theory or have the direct connections with it.)
A. Lande and L. Thomas, Phys. Rev. **60** (1941), 121, 514; Phys. Rev. **65** (1944), 175.
A. Lande, Phys. Rev. **56** (1939), 482; Phys. Rev. **76** (1949), 1176; Phys. Rev. **77** (1950), 814.
B. Podolski et al., Phys. Rev. **62** (1942), 68; Phys. Rev. **65** (1944), 228; Phys. Rev. **67** (1945), 184.
M. Montogomery, Phys. Rev. **69** (1947), 117.
A. E. S. Green, Phys. Rev. **72** (1947), 628; Phys. Rev. **73** (1948), 26.
B. Podolski and P. Schwed, Rev. Mod. Phys. **20** (1948), 40.
L. de Broglie, Comptes Rendus **229** (1949), 157, 269, 401; Phys. Rev. **76** (1949), 862.
H. Bhabha, Phys. Rev. **77** (1950), 665.
2) R. Peierls and H. McManus, Proc. Roy. Soc. **A195** (1948), 323.
3) A. Pais and G. E. Uhlenbeck, Phys. Rev. **79** (1950), 145.
4) E. C. G. Stueckerberg and A. Petermann, Phys. Rev. **82** (1951), 548; Helv. Phys. Acta **24** (1951), 317.
S. Sakata, H. Umezawa and S. Kamefuchi, Phys. Rev. **84** (1951), 154.
5) C. N. Yang and D. Feldman, Phys. Rev. **79** (1950), 972.
6) G. Källén, Arkiv f. fys. **2** nr. (1950), 19.
7) Z. Koba, Prog. Theor. Phys. **5** (1950), 696.
8) R. P. Feynman, Phys. Rev. **74** (1948), 944.
9) W. Pauli and F. Villars, Rev. Mod. Phys. **21** (1949), 434.
10) F. Bopp, ZS. f. Naturforshg. **1** (1946), 53.
M. Born, Rev. Mod. Phys. **21** (1949), 463.
Reference 3) pp. 160.
R. P. Feynman, Phys. Rev. **74** (1948), 939, 1430.

Note added in proof:

After completion of this manuscript, we have seen the paper of J. Rayski (Phil. Mag. **42** (1951), 1289) on the theory of nonlocal interaction. Our opinion differs from him on the problem of the electron self-energy. The difference has been clarified recently by T. Ouchi, and his work will be soon published in this journal.

One of the present authors has recently obtained a theory of the nonlocal field in which the S-matrix has the similar behaviour to that of § 4 in this paper. The outline of that work is reported in this issue. However it contains clumsy and incorrect parts. The corrected full report will be published in the later issue of this journal.

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On the Angular Distribution of D+D Nuclear Reaction Products*

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The anisotropy coefficients of the angular distribution of D+D→H+T reaction products, $I(\theta)=A(1+B\cos^2\theta+C\cos^4\theta)$, are reproduced theoretically by the W.K.B.-method with taking up to incident D-wave and spin-orbit coupling into account in the line of E. J. Konopinski and E. Teller in the higher energy range up to 3.5 Mev.

§ 1. Introduction

In most nuclear transformation problems, especially in the low energy region of incident particles, products particles distribution is generally spherically symmetric in C. M. system.

This general rule had been demonstrated experimentally by e. g. H. Neuert[1] in

$$Li^7+H^1\rightarrow(Be^8)\rightarrow 2\,He^4, \qquad Li^6+D^2\rightarrow(Be^8)\rightarrow H^1+Li^7$$

reactions, where He^4 and H^1 are the product particles as mentioned above. While opposite facts also exist in

$B^{11}+H^1\rightarrow(C^{12})\rightarrow Be^8+He^4$,	(H. Neuert[1])
$D^2+D^2\rightarrow(He^4)\rightarrow H^1+T^3$,	(A. E. Kempton et al.[2])
$\rightarrow n^1+He^3$	(S. Kikuchi et al.[3])
(Bombarding energy E_b: 100–200 kev.)	(H. Neuert[1])

reactions, where the products H^1, n^1 angular distribution in C. M. system are of equatorial plane symmetry having minimum at 90° direction, namely "not isotropic."

These facts show that only S-wave contribution is not sufficient to explain the reactions.

Theoretical considerations of these phenomena have been as follows:

(i) L. Schiff[4]: D+D reactions

Considering $l\neq 0$ waves without spin changes, thus transition characters are

$$^1S\rightarrow{}^1S,\ ^3P\rightarrow{}^3P,\ ^1D\rightarrow{}^1D,\ ^3F\rightarrow{}^3F \text{ etc.}$$

in which higher effects of $l\geqq 2$ are neglected and gets angular distribution formula by the modified Born-approximation method

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$$I(\theta)=A(1+B\cos^2\theta)\ :\ B\sim 0.03,$$

while experiment (H. Neuert[1]) gives

$$I(\theta)=A(1+0.7\cos^2\theta),$$

accordingly theoretical B is too small to match the experiment.

(ii) R. D. Myers[5]

Using the Breit-Wigner's resonance formula in (i) $B^{11}+H^1\rightarrow Be^8+He^4$, gets

$$I(\theta)\sim 1+3\cos^2\theta .$$

This is rather larger than experiment (Neuert[1]) where 1.8 instead of 3. And in (ii) $D^2+D^2\rightarrow H^1+He^3$, considering the excited state of compound nucleus He^4 is $^3P_1$, then

$$I(\theta)\sim 1+\cos^2\theta .$$

This agrees rather well with the experimental coef. 0.7 (Neuert[1]). Still more good is that according to E. Feenberg's calculation[6], $^3P_1$–state of He^4 lies near its dissociation energy and may react without difficulty.

But opposite opinion also exist, that is, if we take $^3P_2$–state as the excited state, then

$$I(\theta)=13+21\cos^2\theta,$$

this is far away in agreement, while there is no reason to abandon $^3P_2$–state. Also it is a defect to use the resonance formula in spite of the fact that the existence of resonance in D+D reaction is doubtful (see 3).

Thereafter experiments have advanced especially in D+D reactions e. g. $D(d,\ p)T^3$ reaction,

R. D. Huntoon[7] (1940), H. P. Manning et al.[8] (1940), E_b : 90～250 kev,
E. Bretcher et al.[9] (1948) 20～ 80 ",
A. Graves[10] (1946) 150～300 ",

$D(d,\ n)He^3$ reaction,

W. E. Bennet[11] (1946) 0.1～3 Mev.

and established

$$I(\theta)=A(1+B\cos^2\theta)\quad \text{in C.M.S.} \qquad (1)$$

where anisotropy coefficient B is an increasing function of energy, while in older days it is regarded as a constant.

This energy dependence of the $B(E)$ is treated theoretically first by E. J. Konopinski and E. Teller[12] (1948) following after the E. Bretcher et al.'s experiment. They taking up to the incident P–waves and spin-orbit coupling in reaction into account, and used the W. K. B. approximation.

But according to the recent experiment of J. M. Blair et al.[13] an alternative formula

$$I(\theta)=A(1+B\cos^2\theta+C\cos^4\theta) \qquad (2)$$

holds in the higher energy region of 1～3.5 Mev. as shown in Table I., where the calculation of E. J. Konopinski and E. Teller does not seem to be sufficient.

Thus the present author[14] has taken up to the D–waves and spin-orbit coupling in their line of calculation, and reproduced the $\cos^4\theta$ distribution theoretically.

Teble I. Coefficients of angular distribution in D+D reaction

E_b (Mev)	$\sigma'=A$ in 10^{-3} b.		B		C	
	H^1	He^3	H^1	He^3	H^1	He^3
1	4	4	0.7	1.7	1.9	1.6
1.5	4.5	4.9	−0.6	0	3.5	3.2
2	4.8	5.6	−1.6	−1.1	4.8	4.4
2.5	5.2	5.7	−2.5	−2.0	5.8	5.3
3	5.7	6.2	−3.3	−2 9	6.7	6.4
3.5	6.0	6 25	−3.8	−3.1	7.6	7.2

§ 2. Characters of transitions and nuclear penetrabilities

Generally, nuclear reactions are ruled by the following selection rules, (i) conservation law (charge numbers, mass numbers, energy and momentum), (ii) angular momentum conservation, (iii) parity conservation, (iv) resultant spin conservation if spin-orbit coupling is weak. Now, two deuterons collide and the total numbers of elementary particles involved are even, thus the total spins are integer, that is, 0 (singlet), 1 (triplet), 2 (quintet). And according to the discussion of Konopinski and Teller we have the following possible transitions :

(i) Spin conservation cases

$$^1S\to{}^1S,\ {}^3P\to{}^3P,\ {}^1D\to{}^1D,\ {}^3F\to{}^3F,\ldots\ldots \qquad (3)$$

(ii) Spin-orbit coupling cases

$$^1S_0\to{}^1S_0,\ {}^3P_2\to{}^3P_2,\ {}^1P_2\to{}^1P_2,\ {}^3P_2\to{}^3F_2,\ {}^1D_2\to{}^1D_2,\ {}^1D_2\to{}^3D_2,\ldots\ldots \qquad (4)$$

for which the author calculate the differential cross section of this reaction.

Here, also, we abondon resonance formula and accept the W. K. B. method or the nuclear penetrabilities $P_l=|e^{-C_l}|^2$, where C_l is given by H. A. Bethe,[15]

$$\frac{C_l}{g}=\frac{1}{2}\frac{1}{\sqrt{\pi}}\left(\frac{1}{2}\pi+\arcsin\frac{1-2x}{\sqrt{1+4xy}}\right)-\sqrt{y+1-x}$$
$$+\sqrt{y}\log\frac{1+2\sqrt{y}\,(\sqrt{y}+\sqrt{y+1-x})}{\sqrt{1+4xy}} \qquad (5)$$

where
$$g^2=\frac{2\mu Z_1Z_2e^2R}{\hbar^2}=M_0R\frac{e^2}{\hbar^2}=2\mu\frac{e^2/R}{\hbar^2}R^2=\left(\frac{R}{\lambda\!\!\!^{-}}\right)^2$$
$$=1/2.053 \quad \text{at } E_b=410 \text{ kev.},$$
$$y=l(l+1)/g^2,$$
$$x=W/B=(\text{relative K. E.})/(\text{barrier height})$$
$$=E_b/2B=E_b/410 \text{ kev.}$$

Using the values

$$2\mu = M_0 = 2M_d = 3.32 \cdot 10^{-24}\,g, \quad e = 4.77 \cdot 10^{-10}\ \text{esu.},$$
$$R = 7 \cdot 10^{-13}\ \text{cm}, \quad \hbar = 1.04 \cdot 10^{-27}\ \text{erg sec.},$$

then, $\quad y_0 = 0,\ y_1 = 4.106,\ y_2 = 12.3,\ y_3 = 24.60.$

Calculated penetrabilities are in Table II.

Table II. Nuclear penetrabilities

x	P_0	P_1	P_2	P_3	$\sqrt{P_0 P_2}$	$\sqrt{P_1 P_3}$
0.1	0.0141	0.00024	$10^{-6} \cdot 0.8$		$10^{-4} \cdot 1.062$	
.2	.1099	.00257	$10^{-5} \cdot 1.57$		$10^{-3} \cdot 1.313$	
.3	.2565	.00802	7.13		4.276	
.4	.4176	.01655	$10^{-4} \cdot 2.03$		9.107	
.5	.5693	.02828	4.10		$10^{-2} \cdot 1.1527$	
.6	.7039	.04221	9.35		2.563	
.7	.7982	.056	$10^{-3} \cdot 1.63$		3.607	
.8	.9054	.071	2.79		5.030	
.9	.9685	.0962	4.33		6.479	
1.0	1	.1176	0.007	0.00004	0.07348	0 0022
1.5		.235	.015	.0003	.124	.0084
2		.375	.027	.0006	.165	.0155
2.5		.519	.042	.0015	.215	.0279
3		.652	.066	.0029	.258	.0427
3.5		.772	.095	.0045	.309	.0589
4		.871	.132	.0075	.364	.0809
4.5		.951	.171	.0122	.414	.1077
5		.996	.215	.0166	.464	.1286
5.5		1	.264	.0227	.514	.1507
6			.315	.0300	.561	.1732
6.5			.369	.0382	.607	.1954
7			.425	.0479	.652	.2188
7.5			.480	.0608	.693	.2466
8			.539	.0750	.734	-2739
8.5			.600	.0900	.775	.3000
9			.652	.1055	.807	.3248
9.5			.706	.1248	.841	.3433
10			.758	.1440	.861	.3495

§ 3. Differential cross sections

According to the line of Konopinski and Teller, we get the following formula for the differential cross section :

(i) Spin-conservation case

$$d\sigma = |\sum a_l \sigma_l^{1/2} g_l^{1/2} Y_{l0}|^2 d\omega \qquad (6)$$

where $\sigma_l = \pi\lambda^2(2l+1)P_l$, $P_l = l\text{-}th$ wave penetrability.

g_l = spin state weight factor, i. e. 1/9, 3/9, 5/9 for singlet, triplet and quintet states,

$|a_l|^2$ = intrinsic (without barrier) nuclear reaction probability which can't be calculated explicitly at this stage, but regarded as adjustable parameters to be determined in future progress,

Y_{l0} = normalized spherical harmonics.

Hence,

$$\begin{aligned} d\sigma = {} & |a_0|^2\sigma_0 g_0 \frac{1}{4\pi} + |a_1|^2\sigma_1 g_1 \frac{3}{4\pi}\cos^2\theta + |a_2|^2\sigma_2 g_2 \frac{5}{4\pi}\,\frac{1}{4}(9\cos^4\theta - 6\cos^2\theta + 1) \\ & + |a_3|^2\sigma_3 g_3 \frac{7}{4\pi}\,\frac{\cos^2\theta}{4}(25\cos^4\theta - 30\cos^2\theta + 9) \\ & + 2|a_1 \cdot a_3|\sqrt{\sigma_1\sigma_3}\sqrt{g_1 g_3}\,\frac{1}{4\pi}\sqrt{21}\,\frac{\cos^2\theta}{2}(5\cos^2\theta - 3)\cos\zeta \\ & - 2|a_0 \cdot a_2|\sqrt{\sigma_0\sigma_2}\sqrt{g_0 g_2}\,\frac{1}{4\pi}\,\frac{\sqrt{5}}{2}(3\cos^2\theta - 1)\cos\chi, \end{aligned} \qquad (7)$$

where $\cos\zeta$, $\cos\chi$ are phase factors of complex multiplications. Substituting the definitions of σ_l, g_l and arranging in the order of $\cos^2\theta$,

$$\begin{aligned} = {} & \frac{d\omega}{4\pi} \cdot \pi\lambda^2\Bigg[\left\{\frac{1}{9}|a_0|^2 \cdot P_0 + \frac{25}{36}|a_2|^2 \cdot P_2 - \frac{5}{9}|a_0 \cdot a_2|\sqrt{P_0 P_2}\cos\chi\right\} \\ & + \left\{3|a_1|^2 P_1 - \frac{150}{36}|a_2|^2 P_2 + \frac{147}{4}|a_3|^2 P_3 \cdot P_3' + \frac{15}{9}|a_0 \cdot a_2|\sqrt{P_0 P_2}\cos\chi\right\}\cos^2\theta \\ & + \left\{\frac{25}{4}|a_2|^2 \cdot P_2 - \frac{245}{2}|a_3|^2 \cdot P_3 \cdot P_3' + 35|a_1 \cdot a_3|\sqrt{P_1 P_3 P_3'}\cos\zeta\right\}\cos^4\theta\Bigg] \end{aligned} \qquad (8)$$

where P_3' is the outgoing F-wave penetrability. Further, this becomes

$$= \frac{d\omega}{4\pi} \cdot \pi\lambda^2 A'\{1 + B\cos^2\theta + C\cos^4\theta\} \qquad (9)$$

where the meanings of A, B and C are clear and the definite functions of a_l's and phase angles.

But, this spin-conservation case can't explain the experiments. This is from the invincible rapidly diverging contribution of $\sim P_2$ term in C, because of lacking of competing P_1 term. So we should like to consider next the spin-orbit coupling case.

(ii) Spin-orbit coupling case

$$d\sigma = |\sum a_{lm} \cdot \sigma_l^{1/2} \cdot g_l^{1/2} \cdot Y_{lm}|^2 d\omega \qquad (10)$$

$$\begin{aligned} = d\omega \Bigg| & \left(\frac{\sigma_0}{9}\right)^{1/2} a_0 Y_{00} + \left(\frac{\sigma_1}{3}\right)^{1/2}\left\{\sum_m a_{1,m} Y_{1,m} + \left(\frac{5}{9} \cdot \frac{1}{2}\right)^{1/2} a_{P_3} Y_{3,-1}\right\} \\ & + \left(\frac{\sigma_2}{9}\right)^{1/2}\sum_m a_{2m} Y_{2m}\Bigg|^2 . \end{aligned} \qquad (11)$$

This can also be arranged as previous, but rather tediously, so only the results are given here,

$$= \frac{d\omega}{4\pi} \cdot \pi\lambda\!\!\!^{-2} A'(1 + B\cos^2\theta + C\cos^4\theta), \tag{12}$$

where

$$\begin{aligned} A &= \pi\lambda\!\!\!^{-2}(P_0 A_0 + P_1 A_1 + P_2 A_2 + \sqrt{P_0 P_2}\, A_{02}) = \pi\lambda\!\!\!^{-2} A', \\ A'B &= P_1 B_1 + P_2 B_2 + \sqrt{P_0 P_2}\, B_{02}, \\ A'C &= P_1 C_1 + P_2 C_2 \end{aligned} \tag{13}$$

and, $A_0 = |a_0|^2/9$,

$$A_1 = \frac{3}{2}(|a_{11}|^2 + |a_{1,-1}|^2) + \frac{35}{32}|a_{PF}|^2 - \frac{1}{4}(|a_{11}\cdot a_{PF}| + |a_{1,-1}\cdot a_{PF}|)\cos\eta,$$

$$A_2 = \frac{25}{36}\left\{|a_{20}|^2 + \frac{3}{2}(|a_{2,2}|^2 + |a_{2,-2}|^2) - \sqrt{6}\,(|a_{20}\cdot a_{22}| + |a_{20}\cdot a_{2,-2}|)\cos\zeta\right\},$$

$$A_{02} = \frac{5}{9}\left\{-|a_0\cdot a_{20}|\cos\chi + \frac{\sqrt{6}}{2}(|a_0\cdot a_{22}| + |a_0\cdot a_{2,-2}|)\cos\xi\right\},$$

$$A'B_1 = 3\left\{|a_{10}|^2 - \frac{1}{2}(|a_{11}|^2 + |a_{1,-1}|^2) - \frac{385}{288}|a_{PF}|^2 + \frac{\sqrt{35}}{2}(|a_{11}\cdot a_{PF}| + |a_{1,-1}\cdot a_{PF}|)\cos\eta\right\},$$

$$A'B_2 = \frac{5}{6}\left\{-|a_{20}|^2 + (|a_{21}|^2 + |a_{2,-1}|^2) - \frac{1}{2}(|a_{22}|^2 + |a_{2,-2}|^2) + \frac{8\sqrt{6}}{3}(|a_{20}\cdot a_{22}| + |a_{20}\cdot a_{2,-2}|)\cos\zeta\right\},$$

$$A'B_{02} = \frac{5}{3}\left\{|a_0\cdot a_{20}|\cos\chi - \frac{\sqrt{6}}{6}(|a_0\cdot a_{22}| + |a_0\cdot a_{2,-2}|)\cos\xi\right\},$$

$$A'C_1 = \frac{5}{4}\left\{\frac{245}{24}|a_{PF}|^2 - \sqrt{35}(|a_{11}\cdot a_{PF}| + |a_{1,-1}\cdot a_{PF}|)\cos\eta\right\},$$

$$A'C_2 = \frac{25}{12}\left\{3|a_{20}|^2 - 2(|a_{21}|^2 + |a_{2,-1}|^2) + \frac{1}{2}(|a_{2,2}|^2 + |a_{2,-2}|^2) - 4\sqrt{6}\,(|a_{20}\cdot a_{22}| + |a_{20}\cdot a_{2,-2}|)\cos\zeta\right\}.$$

These coefficients are also the definite functions of a_{lm}'s and phase angles. Hence, the differential cross section can be regarded as an expansion by nuclear penetrabilities which have been in Table II.

§ 4. The anisotropy coefficients

We should like to search the most suitable values of A, B and C by the least square method, since at this stage we can't get full knowledge to calculate them *a priori*, but of

Table III.

$A=\pi\lambda^2(P_0A_0+P_1A_1+P_2A_2+\sqrt{P_0P_2}\,A_{02})=\pi\lambda^2A'$

E_b (Mev)	x	$\pi\lambda^2$ (barn)	P_0	P_1	P_2	$\sqrt{P_0P_2}$	$A'=A/\pi\lambda^2$	Exp. A (in 10^{-3} b.)	
1	2.44	1.296	1	0.5	0.042	0.205	3.086	H^1 4	He^3 4
1.5	3.66	0.865	1	0.805	0.105	0.325	5.202	4.5	4 9
2	4.88	0.650	1	0.988	0.205	0.45	7.538	4.8	5.6
2.5	6.10	0.520	1	1	0.325	0.57	10.00	5.2	5.7
3	7.32	0.432	1	1	0.465	0.675	12.96	5.7	6.2
3.5	8.54	0.371	1	1	0.605	0.775	15.90	6.0	6.25

(i) $A_0=1.344$, $A_1=1.846$, $A_2=21.08$, $A_{02}=0$ (in 10^{-3})

E_b (Mev)	P_0A_0	P_1A_1	P_2A_2	A'(Cal.)	A (Cal.)
1	1.344	0.9415	0.8009	3.086	4.0
1.5	,,	1.486	2 213	5.043	4.4
2	,,	1.827	4.321	7.492	4.8
2.5	,,	1 846	6.805	10.04	5.2
3	,,	,,	9.801	12.99	5.6
3.5	,,	,,	12.75	15.94	5.9

(ii) $A_0=0.849$, $A_1=1.312$, $A_2=17.86$, $A_{02}=4.400$ (in 10^{-3})

E_b (Mev)	P_0A_0	P_1A_1	P_2A_1	$\sqrt{P_0P_2}\,A_{02}A$	A' (Cal)	A (Cal.)
1	0.849	0.6563	0.6786	0.902	3.086	4.0
1.5	,,	1.0567	1.875	1.421	5.202	4,5
2	,,	1.297	3.661	1.980	7.787	5.1
2.5	,,	1.313	5.804	2.508	10.473	5.4
3	,,	,,	8.304	2.970	13.43	5.8
3.5	,,	,,	10.80	3.410	16.37	6.1

Table IV.

$A'B=P_1B_1+P_2B_2+\sqrt{P_0P_2}\,B_{02}$,

$B_1=5.119$, $B_2=-144.8$, $B_{02}=27.93$ (in 10^{-3})

E_b (Mev.)	Exp. B		$A'B$ (in 10^{-3})	P_1B_1	P_0B_2	$\sqrt{P_0P_2}\,B_{02}$	$A'B$	B (Cal.)
	H^1	He^3		(in 10^{-3})			(in 10^{-3})	
1	0.7	1.7	2.160	2.559	− 6.082	5.726	2.240	0.72
1.5	−0.6	0	− 3.121	4.121	−15.205	9.022	− 2.062	−0.4
2	−1.6	−1.1	−12.061	5.058	−29.687	12.569	−12.059	−1.6
2.5	−2.5	−2.0	−25.000	5.119	−47.065	15.921	−26.023	−2.6
3	−3.3	−2.9	−42.976	,,	−67.339	18.854	−43 369	−3.3
3.5	−3.8	−3.1	−60.594	,,	−87.614	21.648	−60.459	−3.8

Table V.

$A'C = P_1 C_1 + P_2 C_2$,

$C_1 = -4.833$, $C_2 = 197.2$ (in 10^{-3})

E_b (Mev)	Exp. C		$A'C$	$P_1 C_1$	$P_2 C_2$	$A'C$ (Cal.)	C (Cal.)
	H^1	He^3	(in 10^{-3})				
1	1.9	1.6	5.864	−2.416	8.281	5.865	1.9
1.5	3.5	3.2	13.005	−3.890	20.388	16.497	3.3
2	4.8	4.4	36.184	−4.775	40.419	35.685	4.7
2.5	5.8	5.3	58.000	−4.833	64.080	59.147	5.9
3	6.7	6.4	86.851	〃	91.684	86.851	6.7
3.5	7.6	7.2	129.862	〃	119.878	115.045	7.2

course we must check whether they can reproduce the earlier data too and are self-consistent or not. They are listed in Table III, IV, V and the results are compared with the earlier data also using $B+C$ values for H^1 and neutron in Figs. 1 and 2.

There are two best fit sets of A's (i) and (ii) as shown in Table III, of which (ii) seems to give better fit for $B+C$ in the lower energy region as shown in Fig. 3 (where meaningless negative part of C are cut off). While with (i), B values are rather smaller than the earlier experimental data, and A values make rather steeper peak than (ii) (see, Fig. 2).

So, we choose the set (ii) of A, B and C.

Next, we must check whether they are self-consistent or not. For this, inversely solved a_{lm}'s are given as follows;

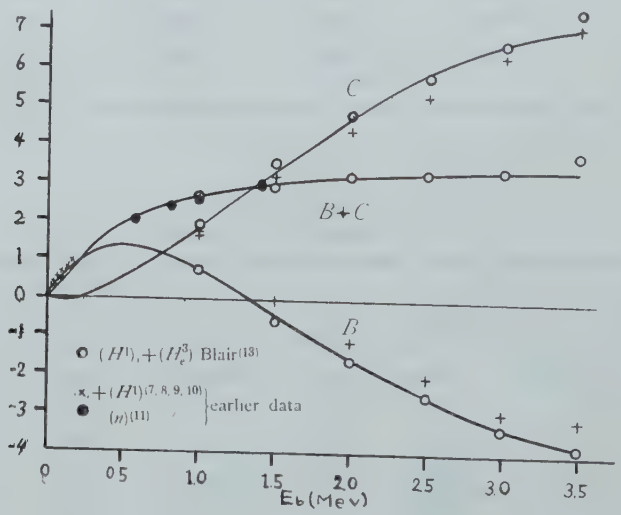

Fig. 1

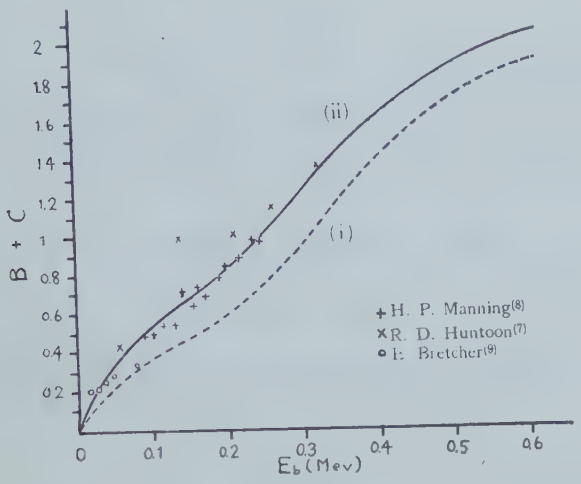

Fig. 2.

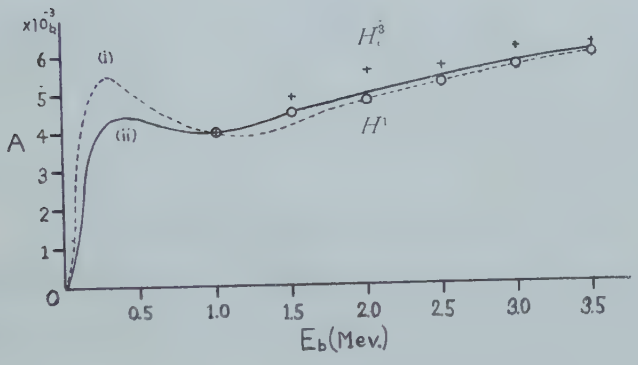

Fig. 3.

$|a_0|^2 = 7.64 \cdot 10^{-3}$,

$0.74 \cdot 10^{-3} < |a_{10}|^2$ and $(|a_{11} \cdot a_{PF}| + |a_{1,-1} \cdot a_{PF}|) < 3.465 \cdot 10^{-3}$,

$0 < (|a_{11}|^2 + |a_{1,-1}|^2) < 0.86 \cdot 10^{-3}$,

$42.6 \cdot 10^{-3} < |a_{20}|^2 < 1$,

$|a_0 \cdot a_{20}| \cos\chi = 27.8 \cdot 10^{-3}$,

$0 < (|a_{22}|^2 + |a_{2,-2}|^2) < 1$ depending on $|a_{20}|^2$,

$|a_0| \cdot (|a_{2,2}| + |a_{2,-2}|) \cos\xi = 29.6 \cdot 10^{-3}$,

$87.2 \cdot 10^{-3} < (|a_{20} \cdot a_{22}| + |a_{20} \cdot a_{2,-2}|) \cos\zeta$,

$10.2 \cdot 10^{-3} < (|a_{21}|^2 + |a_{2,-1}|^2) < 36.5 \cdot 10^{-3}$,

$0 < |a_{PF}|^2 < 0.071 \cdot 10^{-3}$.

Especially, the last shows that the $\cos^6\theta$ term can be neglected. And all these values give the correct signs and the reasonable order of magnitudes.

§ 5. Discussions

We should like to say from the above analysis that

(i) spin-orbit coupling effect is necessary,

(ii) the D–wave contribution and its interference terms are very important, which seems to have interesting relation to the rather large admixture of D–state in the deuteron problem,

(iii) the vanishing of the calculated C at 0.3 Mev corresponds just to Blair et al.'s experimental expect that it happens between $0.5 \sim 1.0$ Mev,

(iv) these $|a_{lm}|^2$s may be servicable to the current theoretical calculation in the future.

At the end the author wishes to thank Prof. K. Umeda for his advice and encouragement.

References

1) H. Neuert, Phys. Z. S. **38** (1937), 122, 618.
2) A. E. Kempton, B. C. Browne and R. Maasdrop, Proc. Roy. Soc. **A157** (1936), 386.
3) S. Kikuchi, H. Aoki and K. Husimi, Proc. Math. Soc. Japan **18** (1936), 35, 188.
4) L. Schiff, Phys. Rev. **51** (1937), 785.
5) R. D. Myers, Phys. Rev. **54** (1938), 361.
6) E. Feenberg, Phys. Rev. **49** (1936), 328.
7) R. D. Huntoon, Phys. Rev. **58** (1940), 77.
8) H. P. Manning, R. D. Huntoon, F. E. Myers and V. J. Young, Phys. Rev. **61** (1941), 371.
9) E. Bretcher, A. P. French and F. G. P. Seidl., Phys. Rev. **73** (1948), 815.
10) E. R. Graves, J. H. Manley and J. H. Coon, Phys. Rev. **70** (1946), 101.
11) W. E. Bennet, C. E. Mandeville and H. T. Richards, Phys. Rev. **69** (1946), 418.
12) E. J. Konopinski and E. Teller, Phys. Rev. **73** (1948), 822.
13) J. M. Blair, G. Freier, E. Lampi, W. Sleator and J. H. Williams, Phys. Rev. **74** (1948), 1599.
14) Y. Nakano, Phys. Rev. **76** (1949), 981.
15) H. A. Bethe, Rev. Mod. Phys. **9** (1937), 178.

Note added in proof

After this calculation was finished (see (14)) several new data and theoretical consideration have appeared e. g.
Experimental:

G. Hunter and H. Richards, E_b 0.49~3.69 Mev. Phys. Rev. **76** (1949), 1445.

K. W. Erickson, J. L. Fowler and E. J. Strovall, Jr., $D(d, n)He$ at 10.3 Mev. Phys. Rev. **76** (1949), 1141.

H. A. Leiter, F. A. Rodgers and P. G. Kruger, Phys. Rev. **78** (1950), 663 at 10 Mev..

Theoretical:

F. M. Beiduk, J. R Pruett, and E. J. Konopinski, Phys. Rev. **77** (1950), 622, 628.

But, very few theoretical and experimental researches especially above 5 Mev. region.

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Some Remarks on the Photo-disintegration of Deuteron, I†

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The photodisintegration process of deuteron is investigated by extrapolating from the low energy side, and the contribution of mesons is also discussed. The singularity of exchange magnetic moments gives some posibility explaining the experiments.

Recent experiments[1,2] on this subjects in high energy region have indicated that there exists a considerable disagreement between the obtained results and the theoretical analysis up to present. That is, the obtained experimental result of total cross section has a slowly decreasing tendency near the incident γ-ray energy $E_\gamma \sim 100$ Mev and becomes almost constant above 140 Mev, contradicting with the rapid drop of the theoretical curve[3)4)]. In this note, we shall point out that the π-meson's effect in nuclear field plays an important role in the high energy photo-reactions and it gives also a possibility to reconcile the above mentioned inconsistency.

§ 1. Extrapolation from the low energy side

For this subjects, Bethe and Peierls[5] have proposed an anticipating work formerly: and after the war, with the advantage of phenomenological treatment of nuclear force in low energy region, Bethe[6] and Bethe & Longmire[7] have treated it dexterously, which was succeeded by Schiff[3] and Marchall-Guth[4] extending to high energies ($\sim$140 Mev).

In high energies, however, one cannot treat the electro-magnetic interaction as sum of the each multipole terms, because the expansion becomes meaningless at $E_\gamma \sim 100$ Mev: in other words, it is favourable to treat it without expansion, or we must at least take into account the higher pole effects. At first, we investigate the contribution of each terms, such as, electric dipole (^3P), intrinsic magnetic dipole (^1S), electric quadrupole (^1D), and magnetic quadrupole (triplet), extrapolating to high energies. (Fig. 1)

As is well known, the obtained result is seriously dependent on the behaviour of wave functions of initial and final states near the origin, which becomes more remarkable with the increase of the energy. We have tentatively used as the wave functions of deuteron ground state the solution of Hulthen Type potential $\psi=(e^{-\alpha r}-e^{-\beta r})/r$.

Electric dipole: In usual, the odd potentials have been understood to be negligible and consequently the (^3P) state to be free. But, the effective potential V_p in P-state

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may vanishe only by the cancellation between ${}^3V_p$ and ${}^1V_p$, as far as indicated from the analysis of scattering process.[8] On the other hand, in the electric dipole transition only ${}^3V_p$ plays a role and so we may obtain the knowledges about ${}^1V_p$ and ${}^3V_p$ separately in the elaborate analysis of the electric dipole transition. The experimental data[9] which indicates the disagreement with the theory even in low energies ($\sim$20 Mev), seems to indicate the nonvanishing ${}^3V_p$ force. Some analysises are now in progress on this point and will appear later. But here, in Fig. 1, curve (A), P-state has been assumed to be free.

Magnetic dipole: As the nuclear force effects seriously in this case, phase shifts and behaviour of the wave function near the origin play a remarkable role even in high energies. Shape independent formula of phase shift is only valid in the energy less than 10 Mev, and is not correct in high energy region even when the higher terms are taken into accounts.

Being used the square-well potential of Christian and Hart,[8] which gives the reasonable phase of the N-P scattering in high energies, the phase shift is calculated. But, for convenience of calculation, we have extrapolated the outside solution to the inside of potential, where the correction at the origin has been made by a factor η. Wave function of final state is, then, $\psi_F=(1-e^{-\eta r})\sin(kr+\delta)$. For the value of factor η, $\eta=3/r_0(=1.28\times10^{+13}\text{cm}^{-1})$ has been used, which was obtained from the low energy scattering data. This expression is not sufficiently accurate in high energies, and have a tendency to increase the total cross section. However, as we have taken the finite range solution in ground state, the change of η does not effect to the cross section considerably, though it is not so small that can be neglected.

Contribution of the Ground ${}^3D$ states: In the case of π-capture by deuteron, it seems that the interference term of S and D states of deuteron has a comparatively dominant effect:[10] however, in our case, its effects are almost negligible for the total cross section (about 3% at $E_\gamma\sim150$ Mev, taking the D-state probability 0.066). For this point, we consider, some more detailed research should be done.

Thus comparing the contributions of electric dipole (curve A in Fig. 1) and quadrupole (curve B) with magnetic dipole (curve C) and quadrupole (curve D), one may easily understand that the contribution of magnetic higher poles may be more dominant in high energies, while in electric transition the dipole term only has an important role, indicating the incorrectness of the expansion. At the energy larger than 200 Mev, the contribution of magnetic poles are in the same order with the electric dipole, and not negligible.

However, its contribution only increases the total cross section as a factor 1.5 at most ($E_\gamma\sim150$ Mev), and is not enough to illustrate the experimental results.

We have also investigated from high energy side, comparing with the extrapolation from the low energy side. The detail will be discussed in the following papers.

§ 2. Contribution of mesons and other effects

At a glance of the experimental data, one may notice that the anomaly occurs at energy about 140 Mev—meson rest mass. Accordingly, it is very likely to consider that

the meson plays an important role in this process. The effects are; (i) real meson production by γ-ray, and succeeding capture by the deuteron and (ii) the interaction between γ-ray and virtual meson current. Other processes, such as (iii) inelastic meson production, (iv) real meson production and disintegration of other deuteron by it, are excluded by experiment which have ascertained the continuance of the proton energy spectrum and its sudden cut at the maximum.

(i) For this process, one can expect the sharp arising of cross section above threshold by γ-π interaction, and have been investigated by Aizu, Kinosita and Miyazawa[11]; but considering the small density of nuclear matter in deuteron, the probability of this capture process by its parent deuteron may be very small. Moreover, it may not explain the anomaly at $E_\gamma \sim 100$ Mev.

(ii) We have calculated as an example the dipole transitions by exchange magnetic moment. As is well known, the present meson theory is perfectly powerless in the description of virtual mesons and so we should take as the exchange magnetic operator that is obtained by phenomenological treatment.[12] But in the expression, there is so much arbitrariness concerning to radial dependency, we feel it difficult to make use of this practically, and have replaced it by one that is proposed from the meson theoretical calculation in the lowest order (P.S. theory).[13]

$$M_{ps}=(e/4\varkappa)(f^2/4\pi)(\varkappa/2M)^2(\tau^{(1)}\times\tau^{(2)})_3\{(\sigma^{(1)}\times\sigma^{(2)})e^{-\varkappa r}$$
$$-((\sigma^{(1)}\times\sigma^{(2)})\cdot\boldsymbol{r})\boldsymbol{r}(1+\varkappa r)e^{-\varkappa r}/r^3\varkappa+(\boldsymbol{r}^{(1)}\times\boldsymbol{r}^{(2)})V_0\},$$

where

$$V_0=1/3\cdot(\sigma^{(1)}\cdot\sigma^{(2)})\varkappa e^{-\varkappa r}/r+S_{12}(1+\varkappa r+\varkappa^2r^2/3)e^{-\varkappa r}/\varkappa r^3. \qquad \text{(I)}$$

This form is consistent with experimental results in the static case such as magnetic moments of ^{3}H, ^{3}He, etc., and not so inreliable. The curve (E) in Fig. 1 shows this contribution, where we take $f^2/4\pi=20$ in (I). Of course, we cannot conclude from this that the virtual mesons have decidedly dominant role, but we may say, at least, there is some possibilities explaining the experiments. But in this results, we should remark here, that, the r-dependency of exchange magnetic operator has affected seriously, and its singularity has given the possibility explaining the experiments, in other word, we can presume that π-mesons may be assembled near the nucleons very closely.

We should express our cordial thanks to the constant advice of Prof. Sakata, and this work is much obliged to the stimulating disscussions with Mr. S. Ogawa, Mr. E. Yamada and Mr. H. Simazu.

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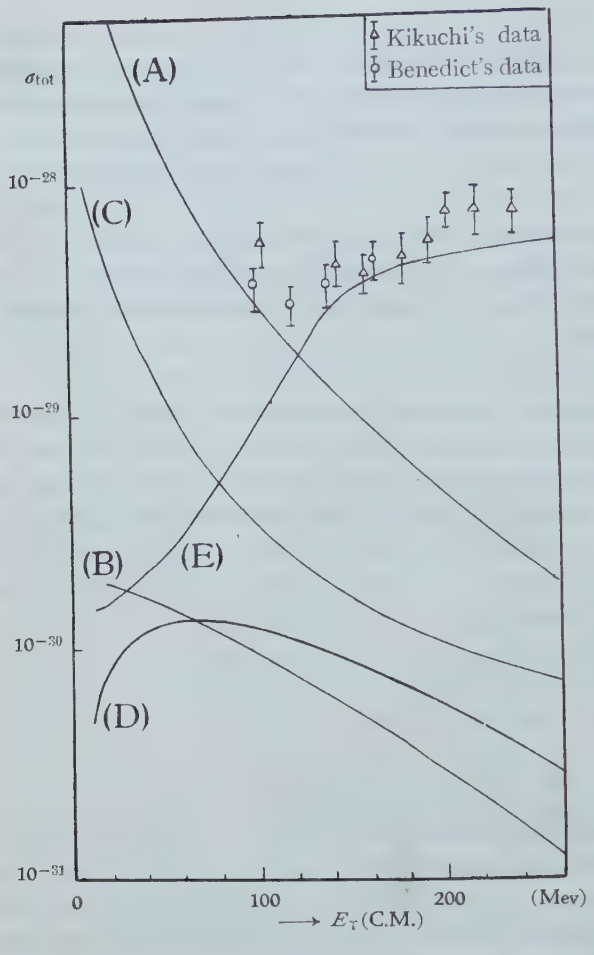

Fig. 1 Total cross sections for electric dipole (A), electric quadrupole (B), magnetic dipole (C), magnetic quadrupole (D), and exchange magnetic moment (E).

References

1) S. Kikuchi, Phys. Rev. **85** (1952), 1062.
2) T. S. Benedict and W. M. Woodward, Phys. Rev. **85** (1952), 924.
3) L. I. Schiff, Phys. Rev. **78** (1950), 733.
4) J. F. Marshall and E. Guth, Phys. Rev. **78** (1950), 738.
5) H. A. Bethe and R. E. Peierls, Proc. Roy. Soc. **A148** (1935), 146.
6) H. A. Bethe, Phys. Rev. **76** (1949), 38.
7) H. A. Bethe and C. Longmire, Phys. Rev. **77** (1950), 647.
8) R. S. Christian and E.W. Hart, Phys. Rev. **77** (1950), 441.
9) E. G. Fuller, Phys. Rev. **76** (1949), 576.
10) G. F. Chew, M. L. Goldberger, J. M. Steinberger and C. N. Yang, Phys. Rev. **84** (1951), 581.
11) K. Aizu, T. Kinosita, and T. Miyazawa, Lecture at the Tokyo Meeting of the Physical Society of Japan, April 1, 1952.
12) R. K. Osborn and L. L. Foldy, Phys. Rev. **79** (1950), 795.
13) S. Ogawa, Lecture at the Kyoto Meeting of the Physical Society of Japan, May 10, 1951.
F. Villars, Phys. Rev. **72** (1947), 256.

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The S Matrix Method in Pion Reactions

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A new method which is convenient for the phenomenological analysis to explore the mutual correlations among various pion reactions is presented based on the S matrix formalism.

We first study the general properties of the S matrix as it is necessary for practical purposes. Next, utilizing the results we discuss the intimate correlations between the photo-meson production and pion-nucleon scattering.

The results seem to be promising in that it can correctly give the ratio:

$$\sigma(\pi^+p)/\sigma(\pi^-p)=3, \qquad \text{(at 130 Mev)}$$

which can never be deduced from the lowest order perturbation theory.

Finally, we apply this method to the qualitative investigation of another process, i.e. the elastic nucleon-nucleon scattering at extremely high energies, from which we can conclude that the scattered nucleons will be concentrated in the forward and backward directions in the centre of mass system.

§ 1. Introduction and summary

From the recent studies on pions, it has already been known that the lowest order perturbation theory cannot even qualitatively predict the correct behaviour of the artificially produced pions. Hence it is a serious problem to consider which kind of method we should rely upon.

In quantum electrodynamics, we have achieved such a remarkable success that allows us consistently to describe the electromagnetic phenomena in terms of the Hamiltonian representing the interaction between electron-positron and electromagnetic fields.

On the other hand, a number of pionic phenomena can hardly be explained in terms of the field theory of mesons.

Although it is suspected that higher order corrections might overcome such a dishonourable situation, yet at present one cannot find a unique Hamiltonian from which one can calculate the matrix elements of all pionic processes with confidence.

Under such circumstances that the present Hamiltonian formalism is not so powerful once applied to pionic phenomena, it is quite probable that the correct theory of pions might be beyond the frame of the Hamiltonian formalism. Thus we shall bear on the S matrix formalism[1)2)] rather than the questionable Hamiltonian formalism, since the former has wider applicability and is more convenient in describing pionic phenomena than the latter. But since we have as yet no concrete means to construct S matrix, we may assume that all conditions satisfied by the S matrix in quantum field theory independently of the special form of the Hamiltonian will hold also in the future theory of S matrix.

One of such conditions is the unitarity of S:

$$S^+S=SS^+=1,$$

where S^+ is the Hermitian conjugate of S.

In section 2, we shall show the special importance of this condition in studying the mutual correlations among various pion reactions. Other conditions such as the invariances of S under Lorentz and gauge transformations are also important. The essence of the content of section 3 consists in these invariance conditions.

In the unitarity condition of S, both S and S^+ appear and the relation between S and S^+ comes into our question. Hence, in section 4, the procedure to derive S^+ from S is investigated in detail.

With these preliminaries, we directly apply the S matrix formalism to the investigation of the mutual correlations among various pion reactions. As an example, a simultaneous integral equation connecting the most important two pionic processes, i.e. the photo-meson production and pion-nucleon scattering, is derived in section 5. From this equation we can calculate the matrix element for the latter provided that those for the former processes are already known. For this purpose, the following properties of pions are necessary to know.

(1) *the transformation properties of pions*

It has already been established from the recent experiments on artificial pions that pions are pseudoscalar.[3]

(2) *the charge dependence of the pion-nucleon interaction*

We assume the most promising and simplest symmetrical theory for the time being. It has long been known that the charge independence of nuclear forces which seems plausible at low energies can be achieved both on the basis of the symmetrical theory and the pure neutral theory and their combinations. However, the symmentrical theory seems superior to other theories such as the pure neutral theory in various processes, though there is yet no definite proof in favour of or against the symmetrical theory.

Perhaps the most promising clue will be gained by the investigation of the process[4]

$$\gamma+d\rightarrow d+\pi^0,$$

since the result predicted from the symmetrical theory shows a marked contrast, to the pure neutral theory, and the recent experimental data seem to show the evidences in favour of the symmetrical theory.

(3) *the possibility of the partial wave expansion*

It must be emphasized that the forces between a pion and a nucleon are of the short range type. This fact guarantees the possibility of treating low energy pionic phenomena by means of the partial wave expansion or synonymously the expansion in energies.

Accordingly we can make use of "the shape independent approximation in meson theory" similar to the phenomenological theory of nuclear forces. As for this point, we shall discuss in section 6.

Regrettably the S matrix method is still impossible to determine the matrix element

of a single process, although it is quite powerful in exploring the mutual correlations among pionic phenomena. Because of this inevitable reason, we must more or less depend on the Hamiltonian formalism, and we shall employ the matrix elements of the photo-meson production derived from a rather phenomenological Hamiltonian, about which we shall discuss in section 7.

In section 8, adopting the matrix elements for the photo-meson production mentioned above to the integral equations, we get those for the pion-nucleon scattering. The result shows a good agreement with the experimental data, especially we obtained the ratio:

$$\sigma(\pi^+ p)/\sigma(\pi^- p)=3, \quad \text{(at 130 Mev)}$$

which can never be deduced from the lowest order perturbation theory. Thus we may say that the phenomenological approach in the field theory is fairly promising at the present stage.

Finally in section 9, we apply this method to nucleon-nucleon collisions at extremely high energies. If the total cross-section of the nucleon-nucleon collisions at extremely high energies is nearly equal to the geometrical cross-section, the angular distribution of the elastic nucleon-nucleon scattering can be deduced, namely the scattered nucleons will be concentrated in the forward and backward directions in the centre of mass system.

§ 2. Unitarity of S matrix

One of the most important properties of S matrix is its unitarity which guarantees the conservation of probability.

Defining the transition matrix R with

$$S=1+R, \tag{2.1}$$

the unitarity of S matrix is expressed by

$$R+R^+ +R^+R=R+R^+ +RR^+=0. \tag{2.2}$$

Now we shall consider the matrix elements of (2) corresponding to the process:

$$\gamma+N\rightarrow N+\pi \qquad \text{(N : nucleon)}. \tag{2.3}$$

Omitting the symbol N for simplicity, we have

$$(\pi|R+R^+|\gamma)+(\pi|R|\pi)\,(\pi|R^+|\gamma)+(\pi|R|\gamma)\,(\gamma|R^+|\gamma) \tag{2.4}$$
$$+\cdots\cdots(\text{higher order terms in } e^2/\hbar c)=0.$$

We cannot apply the perturbation method to the meson-nucleon interaction, but can utilize the power series expansion in terms of the fine structure constant $e^2/4\pi\hbar c=1/\text{“}137\text{”}$. Physically speaking, the γ-ray can be regarded as a test body to investigate the nature of the pion-nucleon interaction, since the photon has so weak interactions with other fields that the perturbation theory holds and its disturbances to other fields can safely be discarded.

Thus picking up only the lowest order terms in the fine structure constant we have from (4)

$$(\pi|R+R^+|\gamma)+(\pi|R|\pi)(\pi|R^+|\gamma)=0. \tag{2.5}$$

This integral equation enables us to derive the matrix elements for pion-nucleon scattering, provided that those for the photo-meson production are already known.

In completely the same way as (4) or (5), we can derive various relations among various pion reactions, but we shall give only one more example. The unitarity relation applied to nucleon-nucleon collisions at energies a little above the threshold of meson production gives

$$(2N|R+R^+|2N)+(2N|R|2N)(2N|R^+|2N) + (2N|R|2N,\pi)(\pi,2N|R^+|2N)=0. \tag{2.6}$$

From this relation, it is easily understood that the total cross-section of pion production can be derived if the matrix elements of (elastic) nucleon-nucleon scattering are known (Cf. § 8,9).

In the present phenomenological theory of nuclear forces, however, we are obliged to make use of real potentials even at high energies, so that the unitarity relation is satisfied by the matrix elements of the elastic scattering only.

$$(2N|R+R^+|2N)+(2N|R|2N)(2N|R^+|2N)=0. \tag{2.7}$$
(phenomenological)

Namely, the contribution from the real meson production is inevitably neglected.

At 340 Mev. we know experimental cross-sections :

reaction	total cross-section
$p+p\to p+p$	$\sim 5\times 10^{-26}$ cm^2,[5]
$p+p\to n+p+\pi^+$	$\sim 2\times 10^{-28}$ cm^2.[6]

It is true that the cross-section of the inelastic collision, i.e. the real meson production is very small compared to the elastic one, but the effect of virtual meson production would convert the nature of the elastic scattering as damping. (See § 9) One can see from the above examples that the S matrix method would be an important clue to explore the correlations among pion reactions.

§ 3. General forms of the transition matrices

In this section, we shall derive such possible forms of matrix elements of R on the basis of the Lorentz and gauge invariances that are convenient for the phenomenological analyses of pions.

The Dirac equation is given in the momentum representation as

$$(i\gamma p+M)\psi(p)=\bar{\psi}(p)(i\gamma p+M)=0, \tag{3.1}$$

where current notations are employed.

The following algebraic relations for the γ matrices are often used throughout this work.

For any four vectors a and b,

$$(\gamma a)(\gamma b)=2(ab)-(\gamma b)(\gamma a), \tag{3.2}$$

and

$$\gamma_\mu(\gamma a)=2a_\mu-(\gamma a)\gamma_\mu,$$

where $\mu=1, 2, 3, 4$.

Making use of (2), the matrix elements of any pion reaction can be reduced to a linear combination of some convenient fundamental forms with simple γ-dependences.[7]

We shall illustrate the fundamental forms by two examples, the photo-meson production and pion-nucleon scattering.

(a) *photo-meson production*

From the requirements of Lorentz and gauge invariances, we have, as the only possible form of the matrix elements of the photo-meson production,

$$(\pi|R|\gamma)\sim\bar{\psi}(F)P_{\mu\nu}(k, I, F, \gamma)\psi(I)A_\mu(k)R_\nu\phi(q), \tag{3.3}$$

where $P_{\mu\nu}$ is an antisymmetric tensor and can be reduced to the linear combination of the following four fundamental forms:

$$\gamma_5(I_\mu F_\nu-I_\nu F_\mu),\quad \gamma_5(\gamma_\mu I_\nu-\gamma_\nu I_\mu), \tag{3.4}$$
$$\gamma_5(\gamma_\mu F_\nu-\gamma_\nu F_\mu),\quad \gamma_5(\gamma_\mu\gamma_\nu-\gamma_\nu\gamma_\mu).$$

We can obtain $P_{\mu\nu}$ by summing up these expressions mutiplied by certain scalar c-numbers It must be noticed that terms appearing in (4) are deduced only for the pseudoscalar theory.

(b) *pion-nucleon scattering*

Assuming the symmetrical theory for pions, the charge dependence of the matrix elements of pion-nucleon scattering is written as

$$\bar{\psi}(F)(Q\tau_{LM}+T\delta_{LM})\psi(I)\phi_L(q_f)\phi_M(q_i)$$

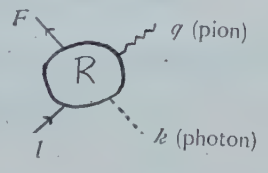


Fig. 1

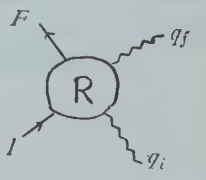


Fig. 2.

where $\tau_{LM}=[\tau_L, \tau_M]/2i$, and the charge dummy indices L and M run from 1 to 3. Next the γ-dependences of Q and T are reduced to

$$Q=Q'(I,F,q_f)+Q''(I,F,q_f)(q\gamma),$$
$$(q=q_i \text{ or } q_f)^* \tag{3.6}$$
$$T=T'(I,F,q_f)+T''(I,F,q_f)(q\gamma).$$

just as in the case of photo-meson production.

Inserting the above reduced forms into the equation (2.5), we obtain a simutaneous integral equation for Q and T.

---

* Notice rhe relation: $\psi(F)(q_i\gamma)\psi(I)=\psi(F)(q_f\gamma)\psi(I)$.

§ 4. Derivation of the conjugate matrix R^+ from R

Since the expression of the unitarity condition of S involves both R and R^+, it is necessary to seek for the procedure to derive R^+ from R. This problem itself is interesting in connection with the principle of detailed balancing.

As readily be seen from the expression

$$(a|R^+|b)=(b|R|a)^*, \qquad (*: \text{complex conjugate}) \tag{4.1}$$

we have to derive matrix element of the inverse process $a\to b$ from that of $b\to a$. Hence we shall investigate the procedure to derive $(b|R|a)$ from $(a|R|b)$. Later on, we shall see that the pseudoscalar character of the pion plays an important rôle in this problem.

First we shall study how to derive the matrix element of the inverse process $\bar{A}$ from the matrix element of a process A based on the Feynman theory.

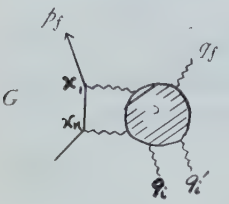


Fig. 3.

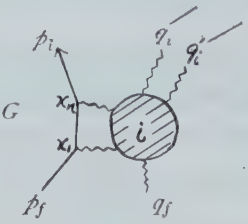


Fig. 4.

diagram G and its in verse diagram G

Let the diagrams corresponding to the process A be G_1, G_2,……, then the sum of contributions from their inverse diagrams $\bar{G}_1$, $\bar{G}_2$, , constitute the matrix element of the inverse process $\bar{A}$. Namely, the diagrams for the processes A and $\bar{A}$ have one-to-one correspondence.

Thus our problem is reduced to a more simplified one how to get a general procedure (common to all diagrams) in order to derive $c(G)$ from $c(G)$, where $c(G)$ means the contribution from a diagram G to S matrix. The diagram $\bar{G}$ is obtained from G by reversing the sense of future and past (See fig. 3 and 4).

The contribution of the diagram G to S matrix is given by

$$c(G)=A\int(dx_1)\cdots\cdots\int(dx_N)e^{-ip_f x_1}\bar{\psi}(p_f)Q_1S_F(x_1-x_2)Q_2\cdots Q_n\psi(p_i)e^{ip_i x_n}$$
$$\times e^{-iq_f x_l}\phi(q_l)e^{iq_i x_m}\phi(q_i')e^{iq_{i'}x_{m'}}, \tag{4.2}$$

where the first line in the integrand corresponds to an open Fermion polygon, and it also stands for other open Fermion polygons if they exist. On the other hand, we need not know the explicit representation of the Boson lines as they are undirected and common to both $c(G)$ and $c(\bar{G})$. A is a numerical factor.

In the meson part, Hermitian ϕ_1, ϕ_2 and τ_1, τ_2 should be used instead of ϕ, ϕ^* and τ, τ^* and summation with regard to the charge dummy indices should be performed. As for the closed Fermion lines, they can be treated as if undirected, for only the sum of contributions from both directions comes into our question.

The contribution of the diagram $\bar{G}$ is given by

$$c(\bar{G})=A\int(dx_1)\cdots\int(dx_N)e^{-ip_i x_n}\bar{\psi}(p_i)Q_n\cdots Q_2S_F(x_2-x_1)Q_1\psi(p_f)e^{ip_f x_1}$$
$$\times e^{-iq_i x_m}\phi(q_i)e^{-iq'_i x'_m}\phi(q_i')\cdots\cdots\phi(q_f)e^{iq_l x_l} \tag{4·3}$$

where the dotted line represents the undirected part common to both $c(G)$ and $c(\bar{G})$. We shall decompose the coupling matrix Q into the direct product of a Dirac matrix O and an isotopic matrix T:

$$Q=O\cdot T. \tag{4·4}$$

T is an Hermitian isotopic matrix such as $1, \tau_1, \tau_2, \tau_3, \tau_P$ as mentioned before.

The problem is how to get (3) from (2).

First we shall apply the following two transformations:

$$\text{(I*)} \qquad \psi(p_i)\to(\bar{\psi}(p_i)C)^T,\ \bar{\psi}(p_f)\to(C^{-1}\psi(p_f))^T. \quad \text{(charge conjugation)} \tag{4·5}$$

$$\phi^{(+)}(q_i)\to\phi^{(-)}(q_f),\ \phi^{(-)}(q_f)\to\phi^{(+)}(q_f).$$

where $(+)$, $(-)$ signs correspond to the positive and negative frequency parts respectively and have been omitted so far in $c(G)$ and $c(\bar{G})$.

$$\text{(II)} \qquad p_i\to-p_i,\ p_f\to-p_f,\ q_i\to-q_i,\ q_f\to-q_f. \tag{4·6}$$

Now let $c(G)$ be changed to $c'(G)$ by these transformations, then making use of the formula

$$C[Q_1S_F(x_1-x_2)Q_2\cdots Q_n]^TC^{-1}=\bar{O}_n\cdots\bar{O}_2S_F(x_2-x_1)\bar{O}_1\cdot T_n^T\cdots T_2^TT_1^T, \tag{4·7}$$

we see

$$c'(G)=A\int(dx_1)\cdots\int(dx_N)e^{-ip_ix_n}\bar{\psi}(p_i)\bar{O}_nT_n^T\cdots\bar{O}_2T_2S_F(x_2-x_1)\bar{O}_1T_1^T\psi(p_f)e^{ip_fx_1}$$
$$\times e^{-iq_ix_m}\phi(q_i)e^{-iq_i'x_m'}\phi(q_i')\cdots\phi(q_f)e^{iq_fx_l}. \tag{4·8}$$

The Boson part in $c'(G)$ agrees completely with that in $c(\bar{G})$.

The only difference is that $Q_n=O_nT_n$ (in $c(\bar{G})$) is replaced by $\bar{O}_nT_n^T$ (in $c'(G)$), where $\bar{O}=CO^TC^{-1}$ and is given in the following table.[8]

We shall compare $c'(G)$ with $c(\bar{G})$ for some special but important cases.

(a) *quantum electrodynamics*

In this case, we can discard the isotopic matrix T, and the only difference is

Tabel of $\bar{O}$

	S	Ps	Pv	V	T	$Pt(T)$
O	1	γ_5	$\gamma_5\gamma_\mu$	γ_μ	$\sigma_{\mu\nu}$	$\gamma_5\sigma_{\mu\nu}$
$\bar{O}$	1	γ_5	$\gamma_5\gamma_\mu$	$-\gamma_\mu$	$-\sigma_{\mu\nu}$	$-\gamma_5\sigma_{\mu\nu}$
Parity	even			odd		

$$O\to\bar{O}. \tag{4·9}$$

* ψ and $\bar{\psi}$ are treated as c-numbers, i.e. commutative but not anticommutative with each other. C is Schwinger's charge conjugation matrix.

In quantum electrodynamics, O is γ_μ(odd), so we have

$$c'(G)=(-1)^N c(\bar{G}). \quad (\text{N: the order of the process})$$

The factor $(-1)^N$ is related only to the parity of the process, i.e. even or odd, and this property is common to all diagrams. Namely

$$\begin{aligned} c'(G)&=c(\bar{G}) \qquad (\text{even order process}) \\ c'(G)&=-c(\bar{G}). \quad (\text{odd order process}) \end{aligned} \tag{4·10}$$

These relations completely settle the solution of our problem in the case of quantum electrodynamics.

(b) *symmetrical meson theory*[9]

In this case, the situation is not so simple as in the former case because of the appearance of isotopic matrices. Yet there is some interting feature. Namely, quite analogous to the charge conjugation matrix C for the Dirac matrices:

$$C^{-1}\gamma_\mu C=-\gamma_\mu^T, \tag{4·11}$$

we can define an isotopic matrix c by

$$c^{-1}\tau_L c=-\tau_L^T. \quad (L=1,2,3) \tag{4·12}$$

For the conventional representation of the isotopic matrices, i,e,

$$\tau_1=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \quad \tau_2=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \quad \tau_3=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},$$

we may choose c as

$$c=\tau_2. \tag{1·13}$$

Thus applying the charge conjugation c in the isotopic space just like the transformation (I) in the ordinary space, we have

$$\text{(III)} \qquad \bar{O}T^T\rightarrow-\bar{O}T. \quad (T=\tau_1,\tau_2,\tau_3) \tag{1·14}$$

Here we have only to apply $c(\ )c^{-1}$ to the isotopic parts lying between $\bar{\psi}(p_i)$ and $\psi(p_f)$.

Let $c'(G)$ be thus changed to $c''(G)$ by the transformation (III), then we have

$$\begin{aligned} c''(G)&=(-1)^N c(\bar{G}) \quad \text{if } O \text{ is even,} \\ c''(G)&= \quad c(\bar{G}) \quad \text{if } O \text{ is odd.} \end{aligned} \tag{4·15}$$

where N(mod. 2), the order of the process, is common to all diagrams as before. (We do not consider the non-linear interactions between nucleon and meson fields.)

In the case of the pseudoscalar meson theory, we can obtain $c(\bar{G})$ by a unified procedure since both pseudoscalar and pseudovector couplings are even, while in the scalar meson theory, we cannot treat both scalar and vector couplings at the same time since they are of different parities.

In view of this difference, we may say that the pseudoscalar theory is a specially convenient case.

(c) *photo-meson production*

What is necessay for our later purpose is the matrix element of the inverse process of the photo-meson production.

We shall give the procedure for only linear terms in the coupling constant e, but the result can also be applied to higher order terms.

The discussion is slightly complicated in this case, because now we have three coexisting fields, nucleonic, mesonic and electromagnetic.

The essential relations in this case are

$$\tau_1{}^T=\tau_1 \quad \tau_2{}^T=-\tau_2, \quad \tau_3{}^T=\tau_3. \tag{4·16}$$

Adopting these relations properly, we are able to get $c(\bar{G})$. For simplicity, we shall assume the symmetrical theory. (This assumption is not necessarily required and the procedure to be shown is also valid for the pure neutral theory.)

The interaction Lagrangian of pseudoscalar meson, nucleon, and radiation fields is given by

$$L_{int}=-if\bar{\psi}\gamma_5\tau_L\psi\cdot\phi_L+ie\bar{\psi}\tau_L\gamma_\mu\psi\cdot A_\mu+eA_\mu(\phi_1\frac{\partial\phi_2}{\partial x_\mu}-\frac{\partial\phi_1}{\partial x_\mu}\phi_2)-\frac{1}{2}e^2A_\mu{}^2(\phi_1{}^2+\phi_2{}^2)\}(ps) \text{ only}$$

$$-i\frac{g}{\varkappa}\bar{\psi}\gamma_5\gamma_\mu\tau_L\psi\cdot\frac{\partial\phi_L}{\partial x_\mu}+\frac{g}{\varkappa}\bar{\psi}\gamma_5\gamma_\mu[\tau_L\tau_P]\psi\cdot A_\mu\phi_L\}(pv) \text{ added.} \tag{4.17}$$

(Natural units $\hbar=c=1$ are employed.)

To this we may add the following Pauli term if necessary:

$$\bar{\psi}\sigma_{\mu\nu}(a_P\tau_P+a_N\tau_N)\psi\cdot F_{\mu\nu}.$$

First we shall study the case of pseudoscalar coupling only, and then prove that the procedure obtained is also valid for the case of pseudovector coupling. In the former case, the photon is absorbed only by the meson or nucleon current, while in the latter case it can also be absorbed by another mechanism through a contact interaction among nucleon, meson, and radiation fields.

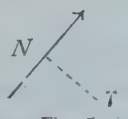


Fig. 5
nucleon current

Fig. 6.
meson current

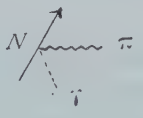


Fig. 7.
contact interaction

The difference of transformation properties in charge space between meson and nucleon fields brings about a positive to negative ratio not equal to unity in the photo-meson production and $\mu_P/\mu_N\neq-1$ in the anomalous magnetic moments of the proton and neutron.

(i) absorption of a photon by the nucleon current

In $c'(G)$, there appears $O\cdot T^T$ corresponding to $O\cdot T$ in $c(\bar{G})$.

When a photon is absorbed by the nucleon current, there is only one vector coupling, i.e. odd γ_μ as O, and in other parts there are only pseudoscalar coupling, i.e. even γ_5.

Thus on the whole, the factor $(-1)^1$ arises from the Dirac part since there is only one odd coupling.

On the other hand, we see that τ_2's in T's changes sign in $c'(G)$ in a manner indicated in (16). Hence, we see

$$c'(G_{nucleon}) = (-1)^{N_2+1} c(\bar{G}), \tag{4·18}$$

where N_2 is the number of τ_2's in $c(G)$.

If we call the pions corresponding to the wave functions ϕ_1, ϕ_2 and ϕ_3, as "1", "2", and "3" pions respectively, virtual "2" pions are always accompanied with τ_2's and contracted in pairs, so that N_2 may be interpreted as the number of "2" pions produced.

The discussion developed above about the interaction $\bar{\psi}\tau_F\gamma_\mu\psi\cdot A_\mu$ can also be applied to the Pauli term $\bar{\psi}\sigma_{\mu\nu}(a_F\tau_F + a_N\tau_N)\psi\cdot F_{\mu\nu}$, for $\sigma_{\mu\nu}$ as well as γ_μ is odd.

(ii) absorption of a photon by the meson current

The expression of the meson current is given by

$$\phi_1\frac{\partial\phi_2}{\partial x_\mu} - \frac{\partial\phi_1}{\partial x_\mu}\phi_2.$$

In this case, all O's are even since no odd matrix exists, so that the factor (-1) does not arise from this Dirac part, but from the isotopic part. For when a photon is absorbed by the meson current, there is always a difference of 1 between the numbers of τ_2's and ϕ_2's, so if N_2 stands for the number of produced "2" mesons as in the case (i), $c'(G)$ due to the meson current can be written as

$$c'(G_{meson}) = (-1)^{N_2+1} c(\bar{G}). \tag{4·19}$$

Since (18) and (19) are of the same form, the general expression for the case of pseudoscalar coupling is given by

$$c'(G) = (-1)^{N_2+1} c(\bar{G}), \tag{4·20}$$

where N_2 is the number of produced "2" mesons.

Next we shall apply this rule to the case with both pseudoscalar and pseudovector couplings.

The discussions about nucleon and meson currents are completely the same with the pseudoscalar coupling case since both pseudoscalar and pseudovector couplings are even. So we shall only be concerned with the contact interaction. The coupling matrix $\gamma_5\gamma_\mu(Pv)$ is even and there is no sign change in the Dirac part, while in the isotopic part, the numbers of τ_2's and ϕ_2's differ by 1, because

$$[\tau_L\tau_P]\phi_L = i(\tau_2\phi_1 - \tau_1\phi_2). \tag{4·21}$$

We thus see the same situation as in the case of the meson current, and the formula (20) is still valid.

That the pseudoscalar and pseudovector couplings have the same parity is very fortunate. This proof can also be applied to other cases such as the pure neutral theory.

It must be noted that we have to transform ϕ_1 and ϕ_2 into ϕ and ϕ^* for practical purposes, which we shall write down for the sake of compltness.

$$\tau^* = (1/2)(\tau_1 - i\tau_2), \quad \tau = (1/2)(\tau_1 + i\tau_2),$$
$$\phi^* = (1/\sqrt{2})(\phi_1 - i\phi_2), \quad \phi = (1/\sqrt{2})(\phi_1 + i\phi_2), \tag{4·22}$$
$$\phi_1 = (1/\sqrt{2})(\phi + \phi^*), \quad \phi_2 = (1/\sqrt{2}\,i)(\phi - \phi^*).$$

Comparing (20) and (22), we see that the factor $(-1)^{N_2}$ is obtained by changing the sign of ϕ_2, leaving ϕ_1 and ϕ_3 unchanged. In other words, the factor is achieved by the following transformation :

(III) $\qquad \phi \to \phi^*, \quad \phi^* \to \phi.$ (charge conjugation) $\qquad (4·23)$

If we denote the expression obtained from $c(G)$ by applying (I), (II) and (III) as $c''(G)$, we have in the case of the photo-meson production

$$c''(G) = -c(\bar{G}). \tag{4·24}$$

With the above procedure, we shall calculate R^+ from R for the case of photo-meson production.

The submatrix corresponding to the photo-meson production can be written as

$$(\pi|R|\gamma) \sim \sum_{s=1}^{4} b_s \bar{\psi}(F) P^s_{\mu\nu} \psi(I) A_\mu(k) k_\nu \phi(q), \tag{4·25}$$

where the coefficients b's are scalar c-numbers, being functions of scalar products of I, F, k and q, and consequently invariant under the transformation (II). P's are given by (3.4).

To apply the transformations (I) and (II) to (25), we have only to replace the P's as

$$P^s \to \epsilon_s P^s, \tag{4·26}$$

where

$$\epsilon_s = \begin{cases} 1, & (s=1) \\ -1. & (s=2,3,4) \end{cases} \tag{4·27}$$

Hence

$$(\gamma|R|\pi) \sim \sum_{s=1}^{4} \epsilon\, b_s \bar{\psi}(F) P^s_{\mu\nu} \psi(I) A_\mu(k) k_\nu \phi(q), \tag{4·28}$$

in which the role of creation and destruction operators should be interpreted in the opposite manner to (25).

Next, from the relation

$$(\pi|R^+|\gamma) = (\gamma|R|\pi)^*,$$

we finally obtain

$$(\pi|R^+|\gamma) \sim \sum_{s=1}^{4} \epsilon_s \eta_s b_s \bar{\psi}(F) P^s_{\mu\nu} \psi(I) A_\mu(k) k_\nu \phi(q), \tag{4·29}$$

where

$$\eta_s = \begin{cases} 1, & (s=4) \\ -1. & (s=1,2,3) \end{cases} \tag{4·30}$$

§ 5. Integral equations

In this section, we shall discuss the integral equations connecting the matrix element of the photo-meson production and that of pion-nucleon scattering.

The elementary photo-meson processes which are experimentally observed are[10]

$$\gamma+p\to p+\pi^0,$$
$$\gamma+p\to n+\pi^+.$$

Corresponding to the above two processes, we have

$$(\pi^0 p|R+R^+|p\gamma)+(\pi^0 p|R|p\pi^0)(\pi^0 p|R^+|p\gamma)+(\pi^0 p|R|n\pi^+)(\pi^+ n|R^+|p\gamma)=0, \tag{5·1}$$

$$(\pi^+ n|R+R^+|p\gamma)+(\pi^+ n|R|p\pi^0)(\pi^0 p|R^+|p\gamma)+(\pi^+ n|R|n\pi^+)(\pi^+ n|R^+|p\gamma)=0. \tag{5·2}$$

which are the concrete expressions of (2·5).

According to the symmetrical theory, the amplitudes of pion-nucleon scattering can be expressed as the linear combinations of two independent quantities Q and T, so that the above two equations are necessary and sufficient to determine the matrix elements of all modes of pion-nuclen scattering.

We shall rewrite ϕ_1 and ϕ_2 by ϕ and ϕ^*, namely

$$\begin{aligned}&(Q\tau_{IM}+T\delta_{IM})\phi_I\phi_M\\&=Q[i\tau_3(\phi\phi^*-\phi^*\phi)+i\sqrt{2}(\tau\phi^*-\tau^*\phi)\phi_3-i\sqrt{2}\phi_3(\tau\phi^*-\tau^*\phi)]\\&+T[\phi\phi^*+\phi^*\phi+\phi_3\phi_3].\end{aligned} \tag{5·3}$$

Then we have only to insert this relation into (1) and (2).

Next, we employ the following normalizations of the wave functions,

$$\begin{aligned}\phi^{(\pm)}(x)&=\frac{1}{\sqrt{2(2\pi)^3}}\int\frac{d\boldsymbol{q}}{q_0}\phi^{(\pm)}(q)e^{\pm iqx},\\\psi^{(+)}(x)&=\frac{1}{\sqrt{2(2\pi)^3}}\int\frac{d\boldsymbol{p}}{p_0}\psi^{(+)}(p)e^{ipx},\\\overline{\psi}^{(-)}(x)&=\frac{1}{\sqrt{2(2\pi)^3}}\int\frac{d\boldsymbol{p}}{p_0}\overline{\psi}^{(-)}(p)e^{-ipx}.\end{aligned} \tag{5·4}$$

which are convenient for covariant calculations.

Then we have

$$\begin{aligned}&<\phi^{(+)}(q)\phi^{(-)}(q')>_0=q_0\delta(\boldsymbol{q}-\boldsymbol{q}'),\\&<\psi(p)\overline{\psi}(p')>_0=(-ip\gamma+M)p_0\delta(\boldsymbol{p}-\boldsymbol{p}').\end{aligned} \tag{5·5}$$

We shall write the transition matrices of the photo-meson production as follows :

$$(\pi^0 p|R|p\gamma) = \int \frac{d\boldsymbol{q}}{q_0}\cdot\frac{d\boldsymbol{F}}{F_0}\cdot\frac{d\boldsymbol{I}}{I_0}\cdot\frac{d\boldsymbol{k}}{k_0}\delta^4(q+F-I-k)$$
$$\times[\sum_s b_s\phi_3(q)\bar{\psi}(F)P^s_{\mu\nu}\tau_P\psi(I)A_\mu(k)k_\nu], \tag{5·6}$$

$$(\pi^+ n|R|p\gamma) = \int \frac{d\boldsymbol{q}}{q_0}\cdot\frac{d\boldsymbol{F}}{F_0}\cdot\frac{d\boldsymbol{I}}{I_0}\cdot\frac{d\boldsymbol{k}}{k_0}\delta^4(q+F-I-k)$$
$$\times[\sum_s a_s\phi^*(q)\bar{\psi}(F)P^s_{\mu\nu}\tau\psi(I)A_\mu(k)k_\nu]. \tag{5·7}$$

Similarly, the transition matrices of the pion-nucleon scattering are

$$(\pi^0 p|R|p\pi^0) = \int \frac{d\boldsymbol{q}_f}{(q_f)_0}\cdot\frac{d\boldsymbol{F}}{F_0}\cdot\frac{d\boldsymbol{I}}{I_0}\cdot\frac{d\boldsymbol{q}_i}{(q_i)_0}\delta^4(q_f+F-I-q_i)$$
$$\times\phi_3(q)\bar{\psi}(F)[T''+T'''(q_i\gamma)]\tau_P\psi(I)\phi_3(q_i),$$

$$(\pi^+ n|R|p\pi^0) = \int \frac{d\boldsymbol{q}_f}{(q_f)_0}\cdot\frac{d\boldsymbol{F}}{F_0}\cdot\frac{d\boldsymbol{I}}{I_0}\cdot\frac{d\boldsymbol{q}_i}{(q_i)_0}\delta^4(q_f+F-I-q_i)$$
$$\times\phi^*(q_f)\bar{\psi}(F)(i\sqrt{2})[Q'+Q''(q_i\gamma)]\tau\psi(I)\phi_3(q_i),$$

$$(\pi^0 p|R|n\pi^+) = \int \frac{d\boldsymbol{q}_f}{(q_f)_0}\cdot\frac{d\boldsymbol{F}}{F_0}\cdot\frac{d\boldsymbol{I}}{I_0}\cdot\frac{d\boldsymbol{q}_i}{(q_i)_0}\delta^4(q_f+F-I-q_i)$$
$$\times\phi_3(q_f)\bar{\psi}(F)(i\sqrt{2})[Q'+Q''(q_i\gamma)]\tau^*\psi(I)\phi(q_i),$$

$$(\pi^+ n|R|n\pi^+) = \int \frac{d\boldsymbol{q}_f}{(q_f)_0}\cdot\frac{d\boldsymbol{F}}{F_0}\cdot\frac{d\boldsymbol{I}}{I_0}\cdot\frac{d\boldsymbol{q}_i}{(q_i)_0}\delta^4(q_f+F-I-q_i)$$
$$\times\phi(q_f)\bar{\psi}(F)[T'+T''(q_i\gamma)-iQ'-iQ''(q_i\gamma)]\tau_N\psi(I)\phi(q_i). \tag{5·8}$$

Inserting the above expressions into (1) and (2), and remembering (5), we reach finally to the integral equations in question.

Next, we must eliminate wave functions such as ψ, $\bar{\psi}$ and A. But notice that the relation

$$\bar{\psi}O\psi=0$$

does not necessarily require

$$O=0.$$

Instead, we have

$$\Lambda(F)O\Lambda(I)=0 \tag{5·9}$$

from

$$\psi(F)O\psi(I)=0,$$

where

$$\Lambda(p)=-ip\gamma+M. \tag{5.10}$$

Similarly we cannot conclude

$$O_{\mu\nu}=0$$

from

$$O_{\mu\nu}A_\mu(k)k_\nu=0. \tag{5·11}$$

In this case, we utilize the result that the S matrix integrated in a covariant manner is equivalent to that integrated after eliminating the longitudinal waves.[11] Namely, we express the electromagnetic potential by the operators which destruct photons with two independent polarizations, and put each coefficient equal to zero.

Then, choosing the direction of $\boldsymbol{k}$ as z-axis, we can rewrite (11) as follows:

$$(\boldsymbol{O}_t)_x+(\boldsymbol{O}_s)_y=0, \qquad (\boldsymbol{O}_t)_y-(\boldsymbol{O}_s)_x=0, \tag{5·12}$$

where

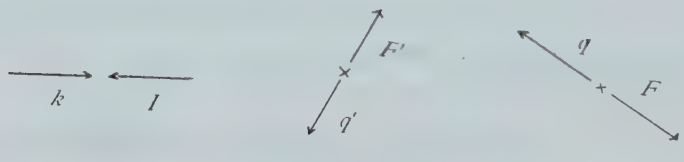
$$\boldsymbol{O}_s=(O_{23}O_{31}O_{12}), \qquad \boldsymbol{O}_t=(O_{10}O_{20}O_{30}).$$

The integrals arising in the matrix multiplications can be reduced to solid angle integrations.

Taking the energy-momentum four vectors in the matrix elements as in fig. 8, we have

$$\int\frac{d\boldsymbol{q}'}{q_0'}\cdot\frac{d\boldsymbol{F}'}{F_0'}\delta^4(q'+F'-F-q)\cdots=\frac{|\boldsymbol{q}|}{q_0+F_0}\int d\Omega(q')\cdots \tag{5·13}$$

Fig. 8.



$$\gamma+N\longrightarrow\pi'+N'\longrightarrow\pi''+N''$$

photo-meson production — pion-nucleon scattering

(Centre of mass system)

We obtain as the final integral equations, after taking traces to eliminate Dirac matrices

$$\begin{aligned}
&\textstyle\sum_s[b_s(q,k)+\varepsilon_s\eta_s b_s^*(q,b)]\mathfrak{A}^s_{\mu\nu}\\
&+\frac{|\boldsymbol{q}|}{q_0+F_0}\int d\Omega_{q'}\Big[\textstyle\sum_s\varepsilon_s\eta_s b_s^*(q',k)\{T'(q,q')\mathfrak{B}^s_{\mu\nu}+T''(q,q')\mathfrak{C}^s_{\mu\nu}\}\\
&\qquad+(i\sqrt{2})\textstyle\sum_s\varepsilon_s\eta_s a_s^*(q',k)\{Q'(q,q')\mathfrak{B}^s_{\mu\nu}+Q''(q,q')\mathfrak{C}^s_{\mu\nu}\}\Big]\equiv 0,\\
&\textstyle\sum_s[a_s(q,k)+\varepsilon_s\eta_s a_s^*(q,k)]\mathfrak{A}^s_{\mu}{}^{s}\\
&+\frac{|\boldsymbol{q}|}{q_0+F_0}\int d\Omega_{q'}\Big[\textstyle\sum_s\varepsilon_s\eta_s(i\sqrt{2})b_s^*(q',k)\{Q'(q,q')\mathfrak{B}^s_{\mu\nu}+Q''(q,q')\mathfrak{C}^s_{\mu}{}^{s}\}\\
&\qquad+\textstyle\sum_s\varepsilon_s\eta_s a_s^*(q',k)\{(T'(q,q')-iQ'(q,q'))\mathfrak{B}_{\mu}{}^{s}_{\nu}\\
&\qquad\qquad+(T''(q,q')-iQ''(q,q'))\mathfrak{C}_{\mu}{}^{s}_{\nu}\}\Big]\equiv 0.
\end{aligned} \tag{5·14}$$

where the equality sign ($\equiv$) means that the equality holds if $\mathfrak{A}_{\mu\nu}$, $\mathfrak{B}_{\mu\nu}$ and $\mathfrak{C}_{\mu\nu}$ in (14) are substituted for in the same way as (12) was obtained from (11). The coefficients a and b are the functions of angles, and $\mathfrak{A}^s_{\mu\nu}$, $\mathfrak{B}^s_{\mu\nu}$ and $\mathfrak{C}^s_{\mu\nu}$ are given by

$$\mathfrak{A}_{\mu\nu}^{s}=Sp[\Gamma\Lambda(F)P_{\mu\nu}^{s}(F,I)\Lambda(I)],$$
$$\mathfrak{B}_{\mu\nu}^{s}=Sp[\Gamma\Lambda(F)\Lambda(F')P_{\mu\nu}^{s}(F',I)\Lambda(I)], \qquad (5\cdot15)$$
$$\mathfrak{C}_{\mu\nu}^{s}=Sp[\Gamma\Lambda(F)(\gamma q)\Lambda(F')P_{\mu\nu}^{s}(F',I)\Lambda(I)],$$

where Γ is an arbitrary Dirac matrix.

The equations (14) are simultaneous Fredholm's integral equations of the first kind. We shall separate these equations.

In the symmetrical theory there are following relations[12]

$$\sqrt{2}\,(\pi^0 p|R|p\pi^0)+(\pi^+ n|R|p\pi^0)=\sqrt{2}\,(\pi^+ p|R|p\pi^+),$$
$$\sqrt{2}\,(\pi^0 p|R|n\pi^+)+(\pi^+ n|R|n\pi^+)=(\pi^+ p|R|p\pi^+), \qquad (5\cdot16)$$

apart from isotopic operators.

Combining (1), (2), and (16), we get

$$\sqrt{2}\,(\pi^0 p|R+R^+|p\gamma)+(\pi^+ n|R+R^+|p\gamma)$$
$$+(\pi^+ p|R|p\pi^+)[\sqrt{2}\,(\pi^0 p|R^+|p\gamma)+(\pi^+ n|R^+|p\gamma)]=0. \qquad (5\cdot17)$$

This is an integral equation for $(\pi^+ p|R|p\pi^+)$ only, so we can first solve this separated equation (17).

It is interesting that the matrix element of pion-nucleon scattering first obtained from those of photo-meson production is relevant to the process $\pi^+ + p\to p+\pi^+$, i.e. the state with charge 2.

We have studied the case of symmetrical theory so far, but we had better discuss here the case of pure neutral theory.

In this case there appear more than two independent amplitudes, and therefore we need informations about

$$\gamma+n\to n+\pi^0, \quad \gamma+n\to p+\pi^-,$$

in addition to the processes

$$\gamma+p\to p+\pi^0, \quad \gamma+p\to n+\pi^+.$$

The complete integral equations are

$$(\pi^0 p|R+R^+|p\gamma)+(\pi^0 p|R|p\pi^0)(\pi^0 p|R^+|p\gamma)$$
$$+(\pi^0 p|R|n\pi^+)(\pi^+ n|R^+|p\gamma)=0,$$
$$(\pi^+ n|R+R^+|p\gamma)+(\pi^+ n|R|p\pi^0)(\pi^0 p|R^+|p\gamma)$$
$$+(\pi^+ n|R|n\pi^+)(\pi^+ n|R^+|p\gamma)=0,$$
$$(\pi^0 n|R+R^+|n\gamma)+(\pi^0 n|R|n\pi^0)(\pi^0 n|R^+|n\gamma)$$
$$+(\pi^0 n|R|p\pi^-)(\pi^- p|R^+|n\gamma)=0,$$
$$(\pi^- p|R+R^+|n\gamma)+(\pi^- p|R|n\pi^0)(\pi^0 n|R^+|n\gamma)$$
$$+(\pi^- p|R|p\pi^-)(\pi^- p|R^+|n\gamma)=0.$$

All the integral equations obtained from (2.5) are given above. Since the matrix elements of inverse processes can be derived from those of original processes by the procedure given in section 4, only independent ones are

(a) $\pi^0+p\rightarrow p+\pi^0$

(b) $\pi^0+n\rightarrow n+\pi^0$

(c) $\pi^++n\rightarrow n+\pi^+$

(d) $\pi^-+p\rightarrow p+\pi^-$

(e) $\pi^0+p\rightarrow n+\pi^+$

(f) $\pi^0+n\rightarrow p+\pi^-$

The charge dependence of the interaction in the pure neutral theory is given by

$$H\sim f(\tau\phi^*+\tau^*\phi)+f_0(1\cdot\phi_0).$$

This interaction is invariant under the substitutions

$$\phi\rightleftarrows\phi^*, \qquad \tau\rightleftarrows\tau^*.$$

The transformation $\tau\rightleftarrows\tau^*$ is achieved by

$$\tau_1^{-1}\tau\tau_1=\tau^*, \quad \tau_1^{-1}\tau^*\tau_1=\tau.$$

Since R is invariant under this transformation

$$R_a=R_b,\ R_c=R_d,\ R_e=R_f.$$

Namely only three of the six transition matrices of $(a),\cdots\cdots,(f)$ are independent, and the four integral equations given above are enough. In this case, however, we can obtain no information on the processes π^++p and π^-+n.

§ 6. Partial wave expansion

In order to solve integral equations, it is convenient to expand T and Q in Legendre polynomials,

$$T(\cos\theta)=\sum_{l=0}^{\infty}T_l\,P_l(\cos\theta). \qquad (6\cdot1)$$

The values of the maximum l's come into question for the purpose of numerical integration, so that we shall roughly evaluate them.

(a) *pion-nucleon scattering*

The interaction between a pion and a nucleon is of short range, if the Coulomb forces are discarded.

Let the impact parameter in pion-nucleon collision be b, then the condition that the collision takes place is given by

$$b < r_f. \quad \text{(force range)} \tag{6·2}$$

The value of r_f is strongly energy dependent for the pseudoscalar pion, but we may regard it as constant in the order of magnitude theory. As the most probable value of r_f, we choose the Compton wave length of pion, i.e.

$$r_f \sim \hbar/\mu c, \tag{6·3}$$

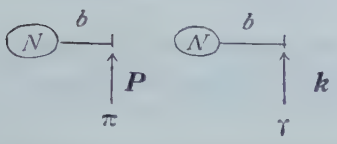


Fig. 9.

Fig. 10.

then the conditions for collision is

$$b \lesssim \hbar/\mu c,$$

with the corresponding angular momentum

$$l\hbar = pb \lesssim p(\hbar/\mu c).$$

Thus the angular momenta which contribute to the scattering are restricted to

$$l \lesssim p/\mu c. \tag{6·4}$$

The correspondence between E and pion angular momentum is tabulated in the following table. (E : meson kinetic energy)

l (in $\hbar$)	1	2	3	4
E(in Mev)	60	170	300	440

(b) *photo-meson production*

In the pion-nucleon scattering, even a low energy incident pion can be scattered, while in the photo-meson production only a photon with energy higher than the threshold can create a pion. So our discussion must be somewhat altered.

The condition that an incident photon with momentum k can create a pion is given by

$$kc \gtrsim \mu c^2. \tag{6·5}$$

Assuming the same force range with the former case, we have

$$l\hbar \lesssim k\frac{\hbar}{\mu c} = \frac{kc}{\mu c^2}\hbar \lesssim \hbar. \tag{6·6}$$

Thus P waves as well as S waves can appear at low energies slightly above the threshold. This fact is surely guaranteed by experiments on $\gamma - \pi^0$ process.

In the above consideration, a photon is treated as though a scalar particle, but it will be enough for such a rough discussion.

As can readily be seen from the above examples, the partial waves that contribute to the process in question are strongly dependent upon the special features of the process.

In pion-nucleon and nucleon-nucleon scatterings, both the initial and final state can be in low energy region, so that only S waves contribute mainly at low energies.

§ 7. Remarks on the photo-meson production

The photo-meson production will be one of the most fundamental reactions among various pionic elementary processes.

In this section, we shall discuss this process from the field theoretical viewpoint.[13]

In the pseudoscalar meson theory, it is well known that the convergence of the perturbation will not be good, but in practice, it is prohibitingly difficult to compute higher order contributions. So some device to take account of the higher order effects has to be performed in a more of less phenomenological manner.

Recently Minami calculated the matrix elements of $\gamma-\pi^0$ upto the order ef^3, and then introduced a Pauli-type interaction phenomenologically in order to estimate the effects of orders higher than ef.[3]

It has already been emphasized that in order to account for the large cross-section of $\gamma-\pi^0$ process the anomalous magnetic moment of a nucleon will play an important rôle, but since the lowest order (ef^2) calculation of anomalous magnetic moment is unsatisfactory we are compelled to introduce this effect in a very complicated way as Minami did.

The Pauli-type interaction can express the effects of the static magnetic moment, but not the non-static effects. Accordingly he calculated the radiative corrections to the Pauli-type interaction.

Thus the orders of the whole expression are

$$ef+cf^3+c\mu'_P f+c\mu'_P f^3, \tag{7·1}$$

where $e\mu'_P f$ is the static anomalous magnetic moment expressing the static effects, and $e\mu'_P f^3$ is expressing the non-static effects.

The results show a fairly good agreement with experimental data, so that we shall employ his matrix elements in the integral equations (5·14).

In practical calculations, the following point should be noticed: in the equation

$$(\pi|R+R^+|\gamma)+(\pi|R|\pi)\,(\pi|R^+|\gamma)=0,$$

the lowest order in the second term is

$$(f^2)\times(ef)=ef^3,$$

therefore the orders that survive in the first term are only

$$ef^3+e\mu_P f^3. \tag{7·2}$$

If there were only terms of order ef^3, our approximation in the calculation of $(\pi|R|\pi)$ would no more be better than the calculation in the lowest order, but since we are assuming that the $c\mu_P f^3$ term expresses phenomenologically the effects of orders higher than ef^3, our approximation will presumably be better than the lowest order calculation.

§ 8. Pion-nucleon scattering

Assuming the matrix elements of $\gamma-\pi$ processes discussed in the previous section, we shall solve the integral equations for the pion-nucleon scattering. Since the matrix elements

of $\gamma-\pi$ processes are given numerically, we must perform numerical integration. For this purpose, the method of partial wave expansion is useful.

As the integral equations concerned are very complicated, we shall illustrate the method by a much simplified example.

The equations in question are Fredholm's integral equations of the first kind and the integration variables are the solid angles.

The simplest equation with the above property is

$$\int f(\cos<\boldsymbol{ab})\,F(\cos<\boldsymbol{bc})\,d\Omega_b=g(\cos<\boldsymbol{ac}), \tag{8·1}$$

where f and g are known functions, and F an unknown function. In order to solve the above equation, expansions in Legendre polynomials are convenient.

$$\begin{aligned} f(\cos\theta)&=\sum f_l\,P_l(\cos\theta),\\ g(\cos\theta)&=\sum g_l\,P_l(\cos\theta),\\ F(\cos\theta)&=\sum F_l P_l(\cos\theta). \end{aligned} \tag{8·2}$$

Choosing the direction of $\boldsymbol{c}$ as the z-axis, we write the polar coordinates of $\boldsymbol{a}$ and $\boldsymbol{b}$ as

$$\boldsymbol{a}:\theta_1,\ 0\,;\qquad \boldsymbol{b}:\theta,\ \varphi \tag{8·3}$$

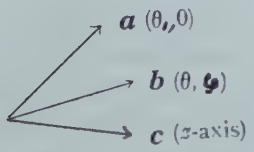


Fig. 11.

Then we have

$$\begin{aligned} \cos<\boldsymbol{ab}&=\cos\theta\ \cos\theta_1+\sin\theta\ \sin\theta_1\ \cos\varphi,\\ \cos<\boldsymbol{bc}&=\cos\theta,\\ \cos<\boldsymbol{ac}&=\cos\theta_1. \end{aligned} \tag{8·4}$$

Next from the addition theorem of Legendre polynomials, we have

$$P_l(\cos<\boldsymbol{ab})=P_l(\cos\theta)\,P_l(\cos\theta_1)+2\sum_{m=1}^{l}\frac{(l-m)!}{(l+m)!}\,P_l^m(\cos\theta)\,P_l^m(\cos\theta_1)\cos m\varphi, \tag{8·5}$$

then substituting this relation into (1), we get from the orthogonality of spherical harmonics

$$F_l=\frac{2l+1}{4\pi}\cdot\frac{g_l}{f_l}$$

$$\text{or}\quad F(\cos\theta)=\sum_l\frac{(2l+1)}{4\pi}\cdot\frac{g_l}{f_l}\cdot P_l(\cos\theta). \tag{8·6}$$

The most serious problem is the convergence of this series, but we assume that it is guaranteed by physical requirements such as the possibility of partial wave expansions discussed in section 6. The equations (5.14) are much more complicated, but the method is essentially the same with the above simplified example.

Next we shall combine the results with Møller's formula for the collision cross-sections.[14]

Suppose that the transition matrix for the pion-nucleon scattering is given by

$$(\pi N|R|N\pi)=\int\frac{d\boldsymbol{q}_i}{(q_i)_0}\cdot\frac{d\boldsymbol{q}_f}{(q_f)_0}\cdot\frac{d\boldsymbol{I}}{I_0}\cdot\frac{d\boldsymbol{F}}{F_0}\delta^4(q_i+I-F-q_f)\bar{\psi}(F)O\psi(I)\phi(q_f)\phi(q_i),\quad(8\cdot7)$$

then refering to the normalizations in section 5, the total cross-section is given by

$$\sigma=\frac{4\pi^2}{\mathfrak{B}}\int\frac{d\boldsymbol{q}_f}{(q_f)_0}\cdot\frac{d\boldsymbol{F}}{F_0}\delta^4(q_i+I-F-q_f)|u(F)Ou(I)|^2,\quad(8\cdot8)$$

with the replacement

$$|u(F)Ou(I)|^2\to\frac{1}{2}S_p(\Lambda(I)O^+\Lambda(F)O).\quad(8\cdot9)$$

Let the differential solid angle representing the direction of $\boldsymbol{q}_f$ be $d\Omega$, then the differential cross-section becomes as

$$\frac{d\sigma}{d\Omega}=\frac{4\pi^2}{\mathfrak{B}}\cdot\frac{|\boldsymbol{q}|}{q_0+F_0}\cdot\frac{1}{2}Sp(\Lambda(I)O^+\Lambda(F)O),\ \text{(in the centre of mass system)}\quad(8\cdot10)$$

where
$$\mathfrak{B}=\sqrt{|\boldsymbol{q}_iI_0-q_{i0}\boldsymbol{I}|^2-|\boldsymbol{q}_i\times\boldsymbol{I}|^2}.\quad(8\cdot11)$$

So the formula (10) is also rewritten as

$$\frac{d\sigma}{d\Omega}=\frac{4\pi^2}{(F_0+q_0)^2}\cdot\frac{1}{2}Sp(\Lambda(I)O^+\Lambda(F)O).\quad(8\cdot12)$$

The matrix O is tabulated in the following.

Table of O

Reaction mode	O
$\pi^++p\to p+\pi^+$	$T+iQ$
$\pi^-+p\to p+\pi^-$	$T-iQ$
$\pi^-+p\to n+\pi^0$	$-i\sqrt{2}Q$

where

$$T=T'+T''(q\gamma),Q=Q'+Q''(q\gamma),$$
$$(q\gamma)^+=-(q\gamma).$$

The total cross-sections can be computed more easily. Combining Møller's formula (8) with the following unitarity conditions:

$$(\pi^+p|R+R^+|p\pi^+)+(\pi^+p|R|p\pi^+)(\pi^+p|R^+|p\pi^+)=0,$$
$$(\pi^-p|R+R^+|p\pi^-)+(\pi^-p|R|p\pi^-)(\pi^-p|R^+|p\pi^-)$$
$$+(\pi^-p|R|n\pi^0)(\pi^0n|R^+|p\pi^-)=0,\quad(8\cdot13)$$

we have for the total cross-section

$$\sigma(\pi N)=-\frac{4\pi^2}{\mathfrak{B}}\cdot\frac{1}{2}Sp[\Lambda(I)(O+O^+)_{\theta=0}],\quad(8\cdot14)$$

where $\theta=0$ means to put the vector $\boldsymbol{q}_f$ equal to $\boldsymbol{q}_i$. Inserting the results obtained by solving the integral equations, we have the total cross-sections of the pion-nucleon scattering, i.e.

$$\left.\begin{array}{l}\sigma(\pi^+p)=105 \ mb \\ \sigma(\pi^-p)=33 \ mb\end{array}\right\} \quad \text{at about 130 Mev (1ab.)} \qquad (8\cdot15)$$

To our regret numerical errors in T and Q are as large as about $10\sim20\%$, so that we cannot calculate differential cross-sections from (8), since (8) is quadratic in T and Q. (But it must be emphasized that the relations (13) are satisfied by our solution within numerical error.) The results, however, bear the following important feature. Its order of magnitude is in good agreement with experiments, especially the ratio

$$\sigma(\pi^+p)/\sigma(\pi^-p)\approx3 \qquad (8\cdot16)$$

is consistent with the recent experimental data[15] even if the numerical errors are taken into account. Remember that this ratio cannot be deduced from the lowest order perturbation theoretical calculations based on the pseudoscalar meson theory with both pseudoscalar and pseudovector couplings.

From this result we may conclude :

Although the effects of higher orders can hardly be estimated in the standard manner, we can still take account of these effects consistently for various pion reactions provided that suitable interactions such as the Pauli term are phenomenologically added.

Another method to describe various pion reactions in a unified manner may be to assume the existence of nucleon isobars and study its effects in pion reactions[16].

§ 9. Elastic nucleon-nucleon collisions at extremely high energies

In previous sections, our interests are limited only to pion reactions at low energies. In contrast to previous sections, we shall now briefly touch upon the problem of nucleon-nucleon collisions at extremely high energies where partial wave analysis is not available.

In this section we shall discuss the correlation between excitation functions and angular distributions of elastic nucleon-nucleon collisions based on the unitary character of S matrix.

Our assumptions in this section are the followings.

(I) *There exists a divergence-free S matrix.*

It is not necessary that this S matrix is constructed from the renormalizable field theory.

(II) *The asymptotic wave functions of particles can be expanded in plane waves.*

The latter assumption is valid only when forces in question are of the short range character, so that Coulomb forces cannot be included.

The fundamental formulas are

$$R+R^+ + RR^+=0, \quad \text{(unitarity)} \qquad (9\cdot1)$$

and Møller's formula.

In nucleon-nucleon collisions at extremely high energies, the multiple production of pions can take place, and possibly also the pair creation of nucleons.

Thus, at extremely high energies we get from (1)

$$-(2N|R+R^+|2N)=(2N|R|2N)\,(2N|R^+|2N) + (2N|R|2N,\pi)\,(\pi,2N|R^+|2N)+\cdots\cdots. \qquad (9\cdot2)$$

From now on we consider the problem in the centre of mass system. Then the total energy of this system is twice the energy of the incident nucleon. At extremely high energies,

$$p_0 = \sqrt{\boldsymbol{p}^2 + M^2} \sim p (= |\boldsymbol{p}|),$$

so we can measure the order of magnitudes of all energies, momenta by the unit p.

Now let the transition matrix for the elastic nucleon-nucleon collision be

$$(2N|R|2N) = \int \frac{d\boldsymbol{p}_f}{(p_f)_0} \cdot \frac{d\boldsymbol{p}_f'}{(p'_f)_0} \cdot \frac{d\boldsymbol{p}_i}{(p_i)_0} \cdot \frac{d\boldsymbol{p}_i'}{(p_i')_0} \delta(p_f + p_f' - p_i - p_i') \bar{\psi}(p_f) \bar{\psi}(p_f') T(p_f, p_f', p_i, p_i') \psi(p_i) \psi(p_i'). \quad (9\cdot 3)$$

Then total cross-section of the elastic collision is given by

$$\sigma_{el} = \frac{4\pi^2}{\mathfrak{B}} \int \frac{d\boldsymbol{p}_f}{(p)^0} \cdot \frac{d\boldsymbol{p}_f'}{(p_f')_0} \delta(p_f + p_f' - p_i - p_i') \frac{1}{4} (Sp)_P (Sp)_N (\Lambda(p_i) \Lambda(p_i') T^+ \Lambda(p_f) \Lambda(p_f') T), \quad \text{for neutron-proton system.} \quad (9\cdot 4)$$

$\mathfrak{B}$ is the relativistic generalization of the relative velocity and becomes here

$$\mathfrak{B} = 2p \cdot p_0.$$

On the other hand the total cross-section including both elastic and inelastic ones is given by

$$\sigma_{total} = -\frac{4\pi^2}{\mathfrak{B}} \cdot \frac{1}{4} (Sp)_P (Sp)_N (\Lambda(p_i) \Lambda(p_i') (T + T^+)_{Q=0}), \quad (9\cdot 5)$$

just as in the previous section.

If there are following relations between $Q(p)$ and $f(p)$,

$$\lim_{p \to \infty} \frac{Q(p)}{f(p)} = \text{finite} \quad (9\cdot 6a)$$

$$\lim_{p \to \infty} \frac{Q(p)}{f(p)} = \text{finite or zero} \quad (9\cdot 6b)$$

then we symbolically write as

$$Q(p) = O(f(p)) \quad (9\cdot 7a), \quad Q(p) \leqq O(f(p)). \quad (9\cdot 7b)$$

And we have

$$\mathfrak{B} = O(p^2), \quad \Lambda = O(p). \quad (9\cdot 8)$$

The total cross-section is the sum of elastic and inelastic ones :

$$\sigma_{total} = \sigma_{el} + \sigma_{inel}, \quad (9\cdot 9)$$

so that it is clearly seen that

$$\sigma_{total} \geqq \sigma_{el}. \quad (9\cdot 10)$$

It is very important that both σ_{total} and σ_{el} in (10) can be expressed in terms of T and T^+ without refering to the precise form of the matrix elements of inelastic collisions. (Cf. (4) and (5))

In the formula (4), T is the function of energy and angle, and the integration is reduced to the one with respect to the solid angle.

Now we assume the energy dependence of T as follows:

$$T=O(f(p)), \tag{9·11}$$

except for the domain of measure zero with regard to the solid angle integration. If we assume that the direction $\theta=0$ does not belong to this exceptional domain, we see from the formulas (4), (5) and (11)

$$\sigma_{el}=O(p^2f^2(p)), \quad \sigma_{total}=O(f(p)). \tag{9·12}$$

Combining (12) with the inequality (10), we get

$$O(f(p))\leqq O(p^{-2}), \tag{9·13}$$

which amounts to

$$\sigma_{total}\leqq O(p^{-2}). \tag{9·14}$$

On the other hand we know from the cosmic ray data that the total cross-section of nucleon-nucleon collision is nearly equal to the geometrical cross-section, i.e.

$$\sigma_{total} \quad \sigma_{geo.}=O(1). \tag{9·15}$$

Accordingly (14) contradicts the experimental data, and we infer that the angle $\theta=0$ indeed belongs to the exceptional domain. Thus

$$T_{\theta=0}>O(f(p)) \quad (9·16a), \text{ or } T_{\theta=0}<O(f(p)). \tag{9·16b}$$

(16b) is also excluded by the same reason with the case

$$T_{\theta=0}=O(f(p)).$$

Therefore we can deduce

$$T_{\theta=0}>O(f(p)).$$

In proton-proton collisions, $\theta=\pi$ also belongs to the exceptional domain. The exceptional domain will perhaps consist of only two angles $\theta=0$ and $\theta=\pi$, since we cannot consider any special angle other than these two.

Thus we can predict the following relation:

$$\lim_{p\to\infty}\left(\frac{d\sigma_{el}}{d\Omega}\right)_\theta\Big/\left(\frac{d\sigma_{el}}{d\Omega}\right)_{\theta=0}=0, \quad (0<\theta<\pi) \tag{9·17}$$

if the effect of Coulomb scattering can be eliminated.

Similar discussions can also be applied to pion-nucleon collisions. In conclusion, the authors express their hearty thanks to Prof. Y. Nambu, Prof. S. Hayakawa and Mr. Y. Yamaguchi for their kind interests taken in this work, and to Mr. S. Minami for his helpful information on the photo-meson production.

References

1) W. Heisenberg, ZS. f. Phys. **120** (1943), 513, 673.
2) C. Møller, Kgl. Danske Vid. Sels. Math-fys. Medd. **23** (1945), 1.
3) a. *spin of the positive pion*
R. E. Marshak, Rev. Mod. Phys. **23** (1951), 137.
W. B. Cheston, Phys. Rev. **83** (1951), 1118.
Durbin, Loar and Steinberger, Phys. Rev. **83** (1951), 646.
Clark, Roberts and Wilson, Phys. Rev. **83** (1951), 649.
b. *parity of the negative pion*
Panofsky, Aamodt and Hadley, Phys. Rev. **81** (1951), 565.
Brueckner, Serber and Watson, Phys. Rev. **81** (1951), 575.
Tamor and Marshak, Phys. Rev. **80** (1950), 766.
c. *spin of the neutral pion*
C. N. Yang, Phys. Rev. **77** (1950), 242.
B. A. Jacobsohn, Bull. Am. Phys. Soc. **27** (1952), No. 1, p. 51.
4) Machida and Tamura, Prog. Theor. Phys. **6** (1951), 572.
Chew and Lewis, Phys. Rev. **82** (1951), 779.
Saito, Watanabe and Yamaguchi, Prog. Theor. Phys **7** (1952), 103.
Heckrotte, Henrich and Lepore, Phys. Rev. **85** (1952), 490.
Francis and Marshak, Phys. Rev. **85** (1952), 496.
5) Chamberlain, Segré and Wiegand, Phys. Rev. **83** (1951), 923.
6) Crawford, Crowe and Stevenson, Phys. Rev. **82** (1951), 97.
Cartwright, Richman, Whitehead and Wilcox, Phys. Rev. **78** (1950), 823; ibid. **81** (1951), 652.
V. Z. Peterson, Phys. Rev. **79** (1950), 407.
Peterson, Iloff and Sherman, Phys. Rev. **84** (1951), 372.
Whitehead and Richman, Phys. Rev. **83** (1951), 855.
7) Koba, Kotani and Nakai, Prog. Theor. Phys. **6** (1951), 849.
8) K. Nishijima, Prog. Theor. Phys. **6** (1951), 614.
9) K. Nishijima, Prog. Theor. Phys. **6** (1951), 1027.
10) Bishop, Steinberger and Cook, Phys. Rev. **80** (1950), 291.
Silverman and Sternes, Phys. Rev. **83** (1951), 853.
11) Coester and Jauch, Phys. Rev. **78** (1950), 149.
Utiyama, Imamura, Sunakawa and Dodo, Prog. Theor. Phys. **6** (1951), 587.
12) W. Heitler, Proc. Roy. Irish. Acad. **51** (1946), 33.
Nambu and Yamaguchi, Prog. Theor. Phys. **6** (1951), 1000.
A similar discussion for the pion-production in nucleon-nucleon collisions was made by Watson and Brueckner, Phys. Rev. **83** (1951), 1.
13) *fourth order corrections*
K. A. Brueckner, Phys. Rev. **79** (1950), 641.
Koba, Kotani and Nakai, see ref. (7).
S. Minami, Prog. Theor. Phys. **7** (1952), 69.
phenomenological introduction of the Pauli moment
Aizu, Fujimoto and Fukuda, Prog. Theor. Phys. **6** (1951), 193.
M. F. Kaplon, Phys. Rev. **83** (1951), 712.
14) See ref. (2), also see
Fukuda and Takeda, Prog. Theor. Phys. **5** (1950), 800.
15) Anderson et al, Phys. Rev. **85** (1952), 936.
16) *photo-meson production*
Fujimoto and Miyazawa, Prog. Theor. Phys. **5** (1950), 1052.
Brueckner and Case, Phys. Rev. **83** (195), 1141.
pion-nucleon scattering
K. A. Brueckner, Phys. Rev. **86** (1952), 106.

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On the Theory of the Green-Functions in Quantum-Electrodynamics

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The re-formulation of Schwinger's theory of Green-functions is carried out by making use of Tomonaga-Schwinger theory. The physical meaning of several quantities and the relations between Green-functions and the S-Matrix are clarified. The general rule for obtaining the Green-functions of many-body problems are derived from our line of reasoning. The removability of divergences arising in the Green-function of one body problem is proved. Ward's identity is derived from the gauge-covariance of Green-functions.

Introduction and summary

Schwinger[1] has recently proposed a theory of Green-functions in quantum-electrodynamics by using his own formalism of quantized fields[2]. His theory is quite attractive and perhaps it will play an important part in the theory of elementary particles, especially in the problems of the so-called "bound-states." His new theory, however, seems somewhat obscure or unsatisfactory concerning the following points:

(1) Spinors $\eta(x)$ and $\bar{\eta}(x)$ are used whose meaning is neither physically obvious nor mathematically comprehensible.

(2) The connections between the Green-functions and the S-Matrix.

(3) The general rule for obtaining the Green-functions of many-body problems.

(4) The investigations concerning the states on the two space-like hypersurfaces σ_1, (where $t_1 = +\infty$) and σ_2 (where $t_2 = -\infty$) on which Schwinger has confined himself only to vacuum states.

(5) The physical meanings of the mass operator M, the polarization operator $P_{\mu\nu}$ and the vertex-operator Γ^{μ}.

(6) The investigation on the possibility of the removal of divergences arising in the several quantities.

(7) The behaviour of the Green-functions and other quantities M, P, etc. under the gauge transformation.

To assist in the further development of this new theory, we try to re-formulate it by using the well-known theory of Tomonaga and Schwinger and to clarify the obscure points mentioned above.

Explaining the line of our reasoning in more detail, we avoid the use of the curious spinors η and $\bar{\eta}$, and start from the Tomonaga-Schwinger equation. Schwinger's Green-

functions G and $\mathfrak{G}$ for the one-body problems are defined in a different way and the fundamental equations satisfied by them are derived under the assumption of expandability in powers of coupling constants. The operators M, $P_{\mu\nu}$ and Γ^{μ} can be understood as the proper self-energy of an electron and a photon, and the proper vertex-part defined respectively by Dyson[3] if we analyse these operators by taking account of the Feynman-Dyson-graphs.

The relation between the Green-functions and the S–matrix can be obtained in the following way. According to Wick's theorem[4] let us expand the S–Matrix into the sum of normal constituents. Then it runs to

$$S/S_{\text{vac}}=1+\int N(\bar{\psi}(y)\psi(y'))\,{}^{(1.0)}M(yy')\,dy\,dy'$$

$$+1/2!\int N(A_{\mu}(y)A_{\nu}(y'))\,{}^{(0.2)}M^{\mu\nu}(yy')\,dy\,dy'+\cdots\cdots,$$

where S_{vac} is $(\text{vac}|S|\text{vac})$. N denotes the normal product. ${}^{(1.0)}M$, ${}^{(0.2)}M^{\mu\nu}$, etc. are C–numbers where the absolute squares are proportional to the transition probabilities in the respective cases. For instance, considering a problem of the radiationless-scattering of an electron by an external field, the element of the S–matrix corsesponding to this process is given by

$$(1,0|S/S_{\text{vac}}|1,0)=(1,0|1|1,0)+\int(1,0|N(\bar{\psi}(y)\psi(y'))|1,0)\,{}^{(1.0)}M(yy')\,dy\,dy'.$$

The suffix (m, n) of the expression $(m, n|S|m', n')$ means that m electron and n photons are present in the final state, and (m', n') has the similar meaning in the initial state. By making use of this notation, S_{vac} can be also expressed as $(0,0|S|0,0)$.

Now we propose to consider the incident electron as being created from the vacuum state by an operator $\psi(x')$ at a world-point $x'(x_0'=-\infty)$, and further the scattered electron as that which will be again annihilated by another operator $\bar{\psi}(x)$ at another world-point $x(x_0=+\infty)$. Explaining this proposal schematically, we consider the problem

$$\underset{\psi(x')\,(x_0'=-\infty)}{\text{vac.}} \longrightarrow \text{an incident electron} \underset{S}{\rightarrow} \text{a scattered electron} \longrightarrow \underset{\bar{\psi}(x)\,(x_0=+\infty)}{\text{vac.}}$$

in place of

$$\text{an incident electron} \underset{S}{\rightarrow} \text{a scattered electron,}$$

that is to say, we are to evaluate

$$(0,0|\psi(\vec{x}, x_0=+\infty)\,S\bar{\psi}(\vec{x'}, x_0'=-\infty)|0,0) \qquad \text{(a)}$$

instead of $(1,0|S|1,0)$. Here it is desirable to generalize this proposal so as to make this procedure applicable not only to the scattering of an electron but also that of a positron, and further to the cases of the pair-creation and annihilation. Furthermore, in order to treat more general cases where the two world-points x and x' are quite arbitrary, we remove the restrictions imposed on the time x_0 and x_0' which are respectively chosen

to be $+\infty$, and $-\infty$ in the above stated cases. The generalized expression of (a) satisfying all the requirements just mentioned above may be written as

$$(\Psi_F^* (\sigma_1 = +\infty)\, T(\psi(x)\bar{\psi}(x')\, S/S_{\text{vac}})\, \Psi_A(\sigma_1 = -\infty)) = (0, 0 \mid T(\psi(x)\bar{\psi}(x')\, S/S_{\text{vac}}) \mid 0, 0)^{*)} \qquad \text{(b)}$$

with $\Psi_A = \Psi_F =$ the vacuum, which seems to us to be the most reasonable. In any way if the quantity (b) can be calculated we are able to know about the element of the S–matrix of the corresponding process. The quantity (b) multiplied by $i = \sqrt{-1}$ is just the Green-function $G(x\,x')$ of the one-electron problem defined by Schwinger.

Now the procedure which makes the problems of evaluating the elements of the S–matrix turn into those of the corresponding Green-functions appears to give rise to superfluous complications by virtue of the operators ψ and $\bar{\psi}$ inserted in the S–matrix. On the other hand, however, it somewhat simplifies the practical calculation of the S–matrix because we are only concerned with those cases where both the initial and final states are vacua. Therefore, we may only calculate such terms in (b) which do not contain any normal product. So far we have been concerned with the interests for the Green-functions from the view point of the practical use, but it will be seen that the Green-function brings about a great advantage in the theoretical investigation on the S–matrix, especially on the removal of divergences arising in it.

Now according to our re-interpretation of the Green-function from the stand-point of the theory of the S–matrix, we can easily define the Green-function of the two-electron problem as follows,

$$G_{12}(x_1 x_2,\, x_1' x_2') = (\Psi_F^*\, T(\psi(x_1)\psi(x_2),\, \bar{\psi}(x_1')\bar{\psi}(x_2')\, S/S_{\text{vac}})\, \Psi_A) \qquad \text{(c)}$$

with $\Psi_A = \Psi_F =$ the vacuum.

Similarly those of the many-electron problems are also easily defined. In this way in the definitions (b) and (c), we have been only concerned with those cases where both the states Ψ_A and Ψ_F prescribed on the two surfaces σ_1 and σ_2 are the vacua. It will be easily seen, however, that the generalized Green-functions defined in the cases where Ψ_A and Ψ_F are not in vacuum state, can be derived from those associated with the vacuous Ψ_A and Ψ_F. Hereafter, let us call the former the generalized Green-function, the latter the "Green function." For instance, consider the generalized Green-function of the one-electron problem associated with the boundary condition in which the states Ψ_A has one ingoing photon and Ψ_F one outgoing photon. This generalized one is given by

$$G^*(x, x') = i(0, 1 \mid T(\psi(x)\bar{\psi}(x')\, S/S_{\text{vac}}) \mid 0, 1) \qquad \text{(b*)}$$

instead of (b), and this can be derived from the Green-function corresponding to the process of Compton-scattering. We believe these remarks are sufficient to show that we may restrict our attention only to the "Green-function," and not to the generalized ones.

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*) Wick's T–product is defined by

$$T(A(x)B(x')) = \theta(x_0 - x_0')A(x)B(x') \pm \theta(x_0' - x_0)B(x')A(x) \begin{cases} +\text{for Bosons,} \\ -\text{for Fermions.} \end{cases}$$

The Green-function corresponding to the process of Compton-scattering can be given by the functional derivative of $G(x, x')$ with respect to the external current J_μ. In general, the Green-function corresponding to the process where m photons and one electron are incident in the initial state, and n photons and one electron are going out in the final state, can be obtained from $G(x, x')$ in the following way;

$$\delta^{m+n}G(x, x')/\delta J_{\mu_1}(\xi_1)\delta J_{\mu_2}(\xi_2)\cdots\cdots\delta J_{\mu_{m+n}}(\xi_{m+n}).$$

In this way, this remark seems to convince us of the situation that we may in principle confine ourselves only to Green-functions corresponding to the process without any photons both in the initial and final states. According to the line of reasoning given by Dyson[6] and Gupta,[7] we can show in a quite simple form, the possibility of the removal of divergences arising in the several quantities. For the success of this proof, Ward's identity is important as Dyson has pointed out which is derived from the covariant character of the mass operator M under the gauge transformation.

§ 1. Relation between Green-functions and the S-matrix

The Lagrangian density in quantum-electrodynamics may be written, with the notations of Schwinger, as

$$L=-\frac{1}{4}F_{\mu\nu}F_{\mu\nu}-\frac{1}{2}\left(\frac{\partial A_\mu}{\partial x_\mu}\right)^2-\bar{\psi}(-i\gamma^\mu\partial_\mu+m)\psi+A_\mu(j_\mu+J_\mu), \qquad (1\cdot1)$$

where

$$\{\gamma_\mu, \gamma_\nu\}=-2\delta_{\mu\nu}(\mu, \nu=1, 2, 3, 4),$$
$$\gamma_0=-i\gamma_4, \quad x_0=-ix_4, \quad \bar{\psi}=\psi^*\gamma_0,$$

ψ^* a complex-conjugate to ψ and J_μ the external current, whereas j_μ is given by

$$j_\mu=\frac{e}{2}\gamma^\mu_{\alpha\beta}(\bar{\psi}_\alpha\psi_\beta-\psi_\beta\bar{\psi}_\alpha).$$

Now let us expand the S-matrix into the sum of normal constituents in the following manner:

$$\begin{aligned}
S/S_{\text{vac}}=1&+\int N(\bar{\psi}(y), \psi(y'))^{(1,0)}M(y, y')\,dy\,dy'\\
&+\int A_\mu(\eta)^{(0,1)}M^\mu(\eta)\,d\eta\\
&+\frac{1}{2!}\int N(A_\mu(\eta), A_\nu(\eta'))^{(0,2)}M^{\mu\nu}(\eta, \eta')\,d\eta\,d\eta' \qquad (1\cdot2)\\
&+\int N(\bar{\psi}(y), \psi(y')A_\mu(\eta))^{(1,1)}M^\mu(y, y', \eta)\,dy\,dy'\,d\eta\\
&+\frac{1}{2!}\int N(\bar{\psi}(y_1)\psi(y_1'), \bar{\psi}(y_2)\psi(y_2'))^{(2,0)}M(y_1y_1', y_2y_2')\,dy_1dy_1'\,dy_2dy_2'\\
&+\cdots\cdots,
\end{aligned}$$

the meaning of the notations $N(\cdots)$, and ${}^{(m,n)}M$ being already explained in the introduction. Elements of the S-matrix of any process can be evaluated by virtue of $(1\cdot2)$, if all the coefficients ${}^{(m,n)}M$ in the expansion $(1\cdot2)$ could be calculated in any way. Consider the radiationless-scattering of an electron by an external field. The element of the S-matrix for this process may be written as

$$(1,0|S/S_{\text{vac}}|1,0)=(1,0|1|1,0)+\int(1,0|N(\bar{\psi}(y)\psi(y'))|1,0)^{(1,0)}M(y,y')\,dy\,dy'. \tag{1\cdot3}$$

Similarly, the element for the transition from one-photon to one-photon is given by

$$(0,1|S/S_{\text{vac}}|0,1)=(0,1|1|0,1)+\frac{1}{2}\int(0,1|N(A_\mu(\eta)A_\nu(\eta'))|0,1)^{(0,1)}M^{\mu\nu}(\eta\eta')\,d\eta\,d\eta'. \tag{1\cdot4}$$

According to the idea stated in the introduction, let us introduce a Green-function $G(x,x')$ of one-electron problem which corresponds to the process $(1\cdot3)$ with the definition

$$G_{\alpha\beta}(x,x')=i(0,0|T(\psi_\alpha(x),\bar{\psi}_\beta(x'),S/S_{\text{vac}})|0,0). \tag{1\cdot5}$$

By means of $(1\cdot2)$ this function runs to

$$G_{\alpha\beta}(xx')=i(0,0|T(\psi_\alpha(x),\bar{\psi}_\beta(x'))|0,0)$$
$$+i\int(0,0|T\{\psi_\alpha(x)\bar{\psi}_\beta(x')N(\bar{\psi}_\rho(y)\psi_\sigma(y'))\}|0,0)^{(1,0)}M_{\rho\sigma}(yy')\,dy\,dy'. \tag{1\cdot6}$$

Remembering the property of T and N products, we can transform the expression $(1\cdot6)$ into

$$G_{\alpha\beta}(x,x')=iS^F_{\alpha\beta}(x-x')+i\int S^F_{\alpha\rho}(x-y)^{(1,0)}M_{\rho\sigma}(yy')S^F_{\sigma\beta}(y'-x')\,dy\,dy' \tag{1\cdot7}^{(*)}$$

or symbolically, we may express as

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*) The contraction of $\psi\bar{\psi}$ and A_μ are given by

$$(\psi_\alpha(x)\bar{\psi}_\beta(x'))=-(\bar{\psi}_\beta(x')\psi_\alpha(x))=S^F_{\alpha\beta}(x-x'),$$
$$(A_\mu(x)A_\nu(x'))=(A_\nu(x')A_\mu(x))=\delta_{\mu\nu}D^F(x-x'),$$

where

$$S^F(x)=(i\gamma^\mu\partial_\mu+m)\Delta^F(x),$$
$$\Delta^F(x)=\frac{1}{2}(\Delta^{(1)}+i\varepsilon(x)\Delta),$$
$$\Delta^{(1)}=\frac{1}{2}(\Delta^+-\Delta^-),\quad \Delta=\frac{-i}{2}(\Delta^+-\Delta^-),$$
$$\Delta^\pm=\frac{1}{(2\pi)^3}\int\frac{d\vec{k}}{\sqrt{\vec{k}^2+m^2}}e^{\pm i(\vec{k}\vec{x}-x_0\sqrt{\vec{k}^2+m^2})}.$$

D^F $D^{(1)}$ D are similarly defined.

S^F and D^F satisfy the equations

$$i\{-i\gamma^\mu\partial_\mu+m\}S^F(x)=\delta(x),$$
$$-i\Box D^F(x)=\delta(x),$$

$$G=iS^F+iS^{F(1,0)}MS^F, \tag{1·7}'$$

if we employ the matrix notations as in Schwinger's paper.

Now the S-matrix may be written as

$$S=\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{\infty}T(H(x_1)\cdots H(x_n))dx_1\cdots dx_n\,;\ H(x)=-A_\mu(j_\mu+J_\mu),$$

provided that the expandability of it in powers of the coupling constant e is assumed. Under the same assumption, the expression (1·4) turns into

$$\begin{aligned}(1,0|S/S_{\rm vac}|1,0)=1/S_{\rm vac}[&(1,0|1|1,0)\\
&-\sum_{n=1}^{\infty}\frac{(-i)^n}{n!}\frac{n!}{1!\,(n-1)!}\int dx\,dx_1\cdots dx_{n-1}(1,0|N(\bar\psi(x)\psi(x))|1,0)\\
&\quad\times(0,0|T(e\gamma^\mu A_\mu(x),H(x_1)\cdots H(x_{n-1}))|0,0)\\
&+\sum_{n=2}^{\infty}\frac{(-i)^n}{n!}\frac{n!}{2!\,(n-2)!}2(1,0|1|1,0)\int dx\,dx'\,dx_1\cdots dx_{n-2}(\bar\psi(x)\psi(x'))\\
&\quad\times\int(0,0|T(eA_\mu(x)\gamma^\mu(x),e\bar\psi(x')\gamma^\mu A_\mu(x'),H(x_1)\cdots H(x_{n-2}))|0,0)\\
&+\sum_{n=2}^{\infty}\frac{(-i)^n}{n!}\frac{n!}{2!\,(n-2)!}2\int dx\,dx'\,dx_1\cdots dx_{n-2}(1,0|N(\bar\psi(x)\psi(x'))|1,0)\\
&\quad\times(0,0|T(eA_\mu(x)\gamma^\mu\psi(x),e\bar\psi(x')\gamma^\mu A_\mu(x'),H(x_1)\cdots H(x_{n-2}))|0,0)]\end{aligned}$$

by virtue of Wick's theorem. The factor $n!/2!(n-2)!$ in the third or fourth term means the number of different ways of choosing arbitrarily two Hamiltonians out of n Hamiltonians $H(x_1),\cdots,H(x_n)$, and the factor 2 in the same term means the number of different ways of taking ψ and $\bar\psi$ out of two Hamiltonians $H(x)$ and $H(x')$ which have been just now chosen out of n H's. These kinds of techniques will be often employed in the following pages. However, we shall omit, hereafter, detailed explanation on these. The factor $(\bar\psi(x)\psi(x'))$ in the third term of the above expression indicates the contraction of $\bar\psi(x)$ and $\psi(x')$ defined by Wick.*) The third term combined with the first term turns into $S_{\rm vac}$.

Bearing in mind the Feynman-graph, we can divide the points $x_1,\cdots x_{n-1}$ in the T-product of the second term into two families of points, one of which contains those connected with the particular point x, and the other the remaining ones not connected with x. Corresponding to this division, the second term turns into

$$\begin{aligned}ieS_{\rm vac}\sum_{n=1}^{\infty}\frac{(-i)^n}{n!}\int&(1,0|N(\bar\psi_\alpha(x),\psi_\beta(x))|1,0)\gamma^\mu_{\alpha\beta}\\
&\times(0|T(A_\mu(x)H(x_1)\cdots H(x_n)|0)_{\rm conn}\,dx\,dx_1\cdots dx_n,\end{aligned}$$

where $S_{\rm vac}$ consists of the sum of contributions from the latter family disconnected with x, and the notation $(|T(\cdots\cdots)|)_{\rm conn}$ will be explained later. Making the similar consideration about the fourth term we get

*) See footnote p. 81.

$$(1,0|S/S_{\text{vac}}|1,0)=(1,0|1|1,0)$$
$$+\int(1,0|N(\bar{\psi}_\alpha(x)\psi_\beta(x'))|1,0)\,dx\,dx'[ie\delta(x-x')\gamma^\mu_{\alpha\beta}\langle A_\mu(x)\rangle$$
$$-\langle T\{eA_\mu(x)(\gamma^\mu\psi'(x))_\alpha e(\bar{\psi}(x')\gamma^\nu)_\beta A_\nu(x')\}\rangle'].\qquad(1\cdot8)$$

The notation $\langle\ \ \rangle$ and $\langle\ \ \rangle'$ employed in (1·8) are defined in the following way. For any operators $A(x)$, $B(y)$, $C(z)$,$\cdots$ in the interaction representation we define $\langle A, B, C,\cdots\rangle$ as

$$\langle A(x), B(y), C(z),\cdots\rangle=\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int(0,0|T\{A, B, C,\cdots H(x_1)\cdots H(x_n)\}|0,0)_{\text{conn}}$$
$$\times dx_1\cdots dx_n\equiv(0,0|T(A, B, C\cdots S/S_{\text{vac}})|0,0).\qquad(1\cdot9)$$

Here $(|T\{\ \ \}|)_{\text{conn}}$ means that in expanding this T-product into the sum of normal constituents we should retain only the terms corresponding to those Feynman-graphs in which every point of $x_1,\cdots,x_n$ is connected, *at least, with one of the particular points* $x, y, z\cdots\cdots$. Similarly we define $\langle A, B, C,\cdots\rangle'$ as

$$\langle A(x), B(y), C(z)\cdots\rangle'=\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}$$
$$\times\int(0,0|T\{A(x), B(y), C(z)\cdots H(x_1)\cdots H(x_n)\}|0,0)'_{\text{conn}}dx_1\cdots dx_n,\qquad(1\cdot9)'$$

where $(|T\{\cdots\}|)'_{\text{conn}}$ has the similar meaning as $(|T\{\cdots\}|)_{\text{conn}}$ with the exception that every points $x_1, x_2,\cdots, x_n$ are connected with all the particular points $x, y, z\cdots\cdots$. Accordingly, all the points $x_1, x_2\cdots x_n, x, y\cdots$ in the expression $(|T\}\cdots\{|)'_{\text{conn}}$ are mutually connected, whereas in $(|T\}\cdots\{|)_{\text{conn}}$ these may be divided into several sets of points in each of which all the points contained in it are mutually connected, however every pair of points separately belonging to different sets is disconnected. In particular from these definitions the following identity holds,

$$\langle A(x), B(y)\rangle=\langle A(x), B(y)\rangle'+\langle A(x)\rangle\langle B(y)\rangle.\qquad(1\cdot9)''$$

From (1·3) and (1·8) we know that

$$^{(1,0)}M_{\alpha\beta}(x, x')=ie\delta(x-x')\gamma^\mu_{\alpha\beta}\langle A_\mu(x)\rangle-\langle eA_\mu(x)(\gamma^\mu\psi(x))_\alpha e(\bar{\psi}(x')\gamma^\nu)_\beta A_\nu(x')\rangle'.\qquad(1\cdot10)$$

Hence, from (1·7) we get

$$G_{\alpha\beta}(x, x')=iS^F_{\alpha\beta}(x-x')-e\int S^F_{\alpha\rho}(x-y)\gamma^\mu_{\rho\sigma}\langle A_\mu(y)\rangle S^F_{\sigma\beta}(y-x')dy$$
$$-i\int S^F_{\alpha\rho}(x-y)\langle eA_\mu(y)(\gamma^\mu\psi(y))_\rho e(\bar{\psi}(y')\gamma^\nu)_\sigma A_\nu(y')\rangle' S^F_{\sigma\beta}(y'-x')dy\,dy'.\qquad(1\cdot11)$$

We shall next consider about the one-photon problem. In the first place, let us evaluate the matrix element

$$(0,1|S/S_{\text{vac}}|0,0)=\int(0,1|A_\mu(x)|0,0)^{(0,1)}M_\mu(x)dx,$$

which can be transformed into

$$i\int (0,1|A_\mu(x)|0,0)\{\langle j_\mu(x)\rangle + J_\mu(x)\}dx,$$

where

$${}^{(0\,1)}M^\mu(x) = i\{\langle j_\mu(x)\rangle + J_\mu(x)\},$$

if we similarly analyse the coefficient ${}^{(0.1)}M^\mu(x)$ as in case of ${}^{(1,0)}M(x, x')$. In quite the same way, we obtain the following;

$$(0,1|S/S_{\text{vac}}|0,1) = (0,1|1|0,1) + \frac{1}{2}\int (0,1|N(A_\mu(x), A_\nu(x'))|0,1)\,{}^{(0.2)}M^{\mu\nu}(x,x')dx\,dx', \tag{1·12}$$

with

$$\begin{aligned}{}^{(0.2)}M^{\mu\nu}(x,x') &= -[\langle j_\mu(x), j_\nu(x')\rangle' + \{\langle j_\mu(x)\rangle + J_\mu(x)\}\{\langle j_\nu(x')\rangle + J_\nu(x')\}] \\ &= {}^{(0.1)}M^\mu(x)\,{}^{(0.1)}M^\nu(x') - \langle j_\mu(x)\, j_\nu(x')\rangle' = {}^{(0.2)}M^{\nu\mu}(x',x).\end{aligned}$$

Corresponding to (1·12), we define the quantity $\mathfrak{K}_{\mu\nu}(xx')$ in the following manner:

$$\begin{aligned}\mathfrak{K}_{\mu\nu}(\xi,\xi') &= i(0|T(A_\mu(\xi), A_\nu(\xi')S/S_{\text{vac}})|0) \\ &\equiv i\langle A_\mu(\xi), A_\nu(\xi')\rangle.\end{aligned} \tag{1·13}$$

This quantity can be written as

$$\mathfrak{K}_{\mu\nu}(\xi,\xi') = i\delta_{\mu\nu}D^F(\xi-\xi') + i\int D^F(\xi-\eta)\,{}^{(0.2)}M^{\mu\nu}(\eta,\eta')D^F(\eta'-\xi')d\eta\,d\eta', \tag{1·14}$$

or in the matrix notation this becomes

$$\mathfrak{K}_{\mu\nu} = i\delta_{\mu\nu}D^F + iD^F\,{}^{0.2)}M^{\mu\nu}D^F. \tag{1·14}'$$

By virtue of (1·12), $\mathfrak{K}_{\mu\nu}$ can be further re-written as

$$\mathfrak{K}_{\mu\nu} = i\delta_{\mu\nu}D^F - iD^F\langle j_\mu, j_\nu\rangle' D^F + i\langle A_\mu\rangle\langle A_\nu\rangle, \tag{1·14}''$$

where the relation

$$\langle A_\mu(x)\rangle = \int D^F(x-y)\,{}^{(0.1)}M^\mu(y)\,dy \tag{1·15}$$

is taken into account.

According to Schwinger, we define the Green-function $\mathfrak{G}_{\mu\nu}$ of the one-photon problem as

$$\mathfrak{G}_{\mu\nu}(x,x') = \mathfrak{K}_{\mu\nu}(x,x') - i\langle A_\mu(x)\rangle\langle A_\nu(x')\rangle. \tag{1·16}$$

Then by means of (1·9)'' and (1·13), we can re-write (1·16) in the simple form such as

$$\mathfrak{G}_{\mu\nu} = i\langle A_\mu, A_\nu\rangle'. \tag{1·16}'$$

It is remarked, in passing, that in case of the one-electron problem we have the expressions

$$G = i\langle\psi\,\psi\rangle = i\langle\psi\,\bar{\psi}\rangle', \tag{1·5}'$$

because of the fact that $\langle\psi\rangle=\langle\bar{\psi}\rangle=0$ holds on account of the conservation of charge.

It is further noted that $\mathfrak{R}$, $\mathfrak{S}$ aud $\langle A_\mu\rangle$ can be represented by

$$\mathfrak{R}_{\mu\nu}(x,x')=\frac{1}{S_{\rm vac}}\frac{\delta}{\delta J_\nu(x')}(S_{\rm vac}\langle A_\mu\rangle)=-i\frac{1}{S_{\rm vac}}\frac{\delta^2 S_{\rm vac}}{\delta J_\mu(x)\delta J_\nu(x')},$$
$$\mathfrak{S}_{\mu\nu}(x,x')=\frac{\delta}{\delta J_\nu(x')}\langle A_\mu(x)\rangle=-i\frac{\delta^2\log S_{\rm vac}}{\delta J_\mu(x)\delta J_\nu(x')}, \qquad (1\cdot17)$$

and

$$\langle A_\mu(x)\rangle=-i\frac{\delta}{\delta J_\mu(x)}\log S_{\rm vac}.$$

In concluding this section, we shall give some remarks about the generalized Green-function G^* of one-electron problem defined by (b^*), namely,

$$G^*(x,x')=i(0,1|T(\psi(x)\bar{\psi}(x')S/S_{\rm vac})|0,1).$$

By taking account of the expansion $(1\cdot2)$, G^* turns into

$$G^*=(0,1|1|0,1)G(x,x')+\frac{i}{2}\int(0,1|N(A_\mu(\xi),A_\nu(\xi'))|0,1)d\xi d\xi'$$
$$\times[S^F(x-x')^{(0,2)}M^{\mu\nu}(\xi,\xi')+\int S^F(x-y)^{(1,2)}M^{\mu\nu}(yy',\xi\xi')S^F(y'-x')dy\,dy'].$$
$$(1\cdot18)$$

Introduce the quantities ${}^{(m,n)}M'$ associated with ${}^{(m,n)}M$ in the following way:

$$^{(1,1)}M'^{\mu}(x,x',\xi)={}^{(1,1)}M^{\mu}(x,x',\xi)-{}^{(1,0)}M(x,x')^{(0,1)}M^{\mu}(\xi),$$
$$^{(0,2)}M'^{\mu\nu}(\xi,\xi')={}^{(0,2)}M^{\mu\nu}(\xi,\xi')-{}^{(0,1)}M^{\mu}(\xi)\,{}^{0,1}M^{\nu}(\xi'),$$
$$^{(1,2)}M'^{\mu\nu}(xx',\xi\xi')={}^{(1,2)}M^{\mu\nu}(xx',\xi\xi')-{}^{(1,0)}M(x,x')^{(0,2)}M^{\mu\nu}(\xi,\xi')$$
$$-{}^{(1,1)}M^{\mu}(xx'\xi)^{(1,0)}M^{\nu}(\xi')-{}^{(1,1)}M'^{\nu}(xx'\xi')^{(0,1)}M^{\mu}(\xi),$$
$$\cdots\cdots\cdots

Let us define the Green-functions corresponding to the Bremsstrahlung and Compton-scattering as

$$B_\mu(xx'\xi)=\partial G(x,x')/\partial J_\mu(\xi)=-\langle\psi(x)\bar{\psi}(x')A_\mu(\xi)\rangle',$$
$$C_{\mu\nu}(xx',\xi\xi)=\delta^2 G(x,x')/\delta J_\mu(\xi)\delta J_\nu(\xi')=-i\langle\psi(x)\bar{\psi}(x')A_\mu(\xi)A_\nu(\xi')\rangle. \quad (1\cdot20)$$

Bearing in mind the definitions $(1\cdot9)$, $(1\cdot9)'$ and using the relations $(1\cdot19)$, we can transform $(1\cdot20)$ into

$$B_\mu(xx'\xi)=-\int S^F(x-y)D^F(\xi-\xi')^{(1,1)}M'^\mu(yy'\xi')S^F(y'-x')\,dy\,dy'\,d\xi',$$
$$C_{\mu\nu}(xx'\xi\xi')=-i\int S^F(x-y)D^F(\xi-\eta)^{(1,2)}M'^{\mu\nu}(yy',\eta\eta')D^F(\eta'-\xi')$$
$$\times S^F(y'-x')\,dy\,dy'\,d\eta\,d\eta'. \quad (1\cdot20)'$$

Therefore the problem of evaluating the generalized Green-function G^* may be reduced to that of evaluating G, $\mathfrak{S}_{\mu\nu}$, B_μ, $C_{\mu\nu}$. Thus we may restrict our attention only to the Green-functions associated with the vacuum states without any loss of generality.

§ 2. Green-function of the one-electron problem

The Green-function $G(x,x')$ of the one-electron problem is defined by $(1\cdot5)'$, namely,

$$G_{\alpha\beta}(xx')=i\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int(0,0|T\{\psi_\alpha(x),\bar{\psi}_\beta(x'),H(x_1)\cdots H(x_n)\}|0,0)'_{\mathrm{conn}}\,dx_1\cdots dx_n. \quad (2\cdot1)$$

The operator $\psi_\alpha(x)$ in $(2\cdot1)$ forms a contraction with $\bar{\psi}_\beta(x')$ or with another $\bar{\psi}$ contained in one of n H's. Corresponding to these two cases, we may transform $(2\cdot1)$ into the sum of two parts in the following manner;

$$G=i(\psi_\alpha(x)\bar{\psi}_\beta(x'))-i\sum_{n=1}^{\infty}\frac{(-i)^n}{n!}\cdot n\cdot\int(0,0|T(\psi_\alpha(x)\bar{\psi}_\rho(y))|0,0)dy$$
$$\times\int(0,0|T\{eA_\mu(y)(\gamma^\mu\psi(y))_\rho,\bar{\psi}_\beta(x'),H(x_1)\cdots H(x_{n-1})\}|0,0)'_{\mathrm{conn}}\,dx_1\cdots dx_{n-1}$$
$$=i(\psi_\alpha(x)\bar{\psi}_\beta(x'))-\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int(\psi_\alpha(x)\bar{\psi}_\rho(y))$$
$$\times\int(0,0|T\{eA_\mu(y)(\gamma^\mu\psi(y))_\rho,\bar{\psi}_\beta(x'),H(x_1)\cdots H(x_n)\}|0,0)'_{\mathrm{conn}}\,dy\,dx_1\cdots dx_n. \quad (2\cdot2)$$

For convenience, we shall use in the following pages a term "a graph of a T-product," by which will be meant a Feynman-graph corresponding to any one of the normal constituents arising in the Wick's expansion of that T-product. As already stated, all the points $x_1,\cdots,x_n$ in every allowable graph of the T-product in $(2\cdot2)$ are connected with each other and particular points y and x' by photon lines or electron lines. In every such graph there is always a photon line called λ and an electron line called λ' both incident

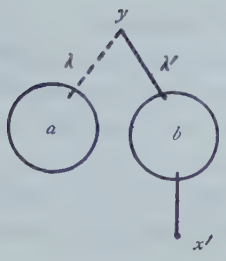

Fig. 1

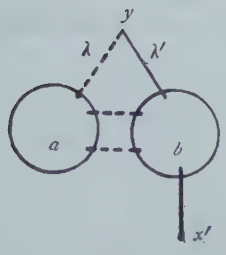

Fig. 2

at the particular point y. (Fig. 1) Consider now the two cases defined in the following way :

1st case

The points $x_1, \cdots, x_n$ may be divided into two sets of points a and b defined in such a way that every point in a can not be connected with y without passing through the particular photon line λ, and the set b contains the remaining points which are connected with y by passing along the particular line λ'. The particular point x' must be connected with the points in b without passing along λ on account of the conservation of charge. (Fig. 1)

2nd case

All the points $x_1, \cdots, x_n$ can not be divided into two sets as in the above stated way. (Fig. 2) That is to say, every point of $x_1, \cdots, x_n$ can be connected with y by passing not only through the line λ but also through λ'. Accordingly every point can be connected with x' without passing through the line λ. (Fig. 2)

Corresponding to these two cases, the second term in (2·2) may be transformed into

$$-\int dy\, S^F_{\alpha\rho}(x-y)\, c\gamma^\mu_{\rho\sigma} \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int (0,0|T\{A_\mu(y), H(y_1)\cdots H(y_n)\}|0,0)_{\text{conn}}\, dy_1\cdots dy_n$$

$$\times \sum_{m=0}^{\infty} \frac{(-i)^m}{m!} \int (0,0|T\{\psi_\sigma(y), \bar{\psi}_\beta(x'), H(x_1)\cdots H(x_m)\}|0,0)'_{\text{conn}}\, dx_1\cdots dx_m$$

$$-\int S^F_{\alpha\rho}(x-y) \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int (0,0|T\{e A_\mu(y)(\gamma^\mu\psi(y))_\rho \bar{\psi}_\beta(x'),$$

$$H(x_1)\cdots H(x_n)\}|0,0)'_{\text{conn (case II)}}\, dy\, dx_1\cdots dx_n . \qquad (2\cdot3)$$

In expanding the T-product of the second term in (2·3) into the sum of normal constituents, we should retain only the terms corresponding to the second case shown in Fig. 2. The first term of (2·3) may be written simply as

$$ie\int \{S^F(x-y)\gamma^\mu \langle A_\mu(y)\rangle G(y,x')\}_{\alpha\beta}\, dy,$$

provided that the definitions (2·1) and (1·9) are used.

Let us next analyse the second term of (2·3) in more detail. For brevity, we use a term "bridge-line" with the definition that when any Feynman-diagram is divided into two pieces joined by a single line, this line is called a bridge-line. Suppose now that an electron-bridge-line is chosen out of any one of allowable graphs of the last T-product in (2·3) where n is supposed to be fixed. Then this diagram is divided into two pieces α and β. The points in α can not be connected with x' without crossing the bridge, and the set β contains only the remaining points. (Fig. 3)

Particularly the set β is empty when this bridge happens to agree with λ_2.

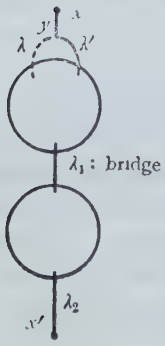

Fig. 3

However, in general, there may be several bridge-lines. The number of points in β changes in conformity with the situation that which bridge-line is chosen out. Now let us choose a particular bridge-line so as to make β to be the maximal set, and call this bridge-line λ_1.

Then the set α combined with λ and λ' turns into an ordinary proper self-energy part of the $(k+2)$-th order in the coupling constant e, where $(k+1)$ is the number of points in α.

Making similar considerations about all the allowable constituents appearing in the second term of (2·3), and summing up over all the contributions from the sets α's and β's separately, we can finally write down the second expression in (2·3) as,

$$\int S^F_{\alpha\rho}(x-y)\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\cdot n\cdot\sum_{\substack{k=0\\(k+l=n-1)}}^{n-1}\frac{(k+l)!}{k!\,l!}\int(0,0|T\{eA_\mu(y)(\gamma^\mu\psi(y))_\rho$$
$$\times H(x_1)\cdots H(x_k),\ e(\bar\psi(z)\gamma^\nu)_\sigma A_\nu(z)\}|0,0)'_{\text{conn, prop}}$$
$$\times(0|T\{\psi_\sigma(z)H(z_1)\cdots H(z_l)\bar\psi_\beta(x')\}|0)'_{\text{conn}}dy\,dz\,dx_1\cdots dx_k dz_1\cdots dz_l\,.$$

Here, the notation $(0|T(\cdots)|0)'_{\text{conn, prop}}$ means that we should retain only those terms which correspond to connected and proper graphs of this T-product. Putting

$$\sum^*_{\alpha\beta}(x,x')=-ie^2\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int(0,0|T\{A_\mu(x)(\gamma^\mu\psi(x))_\alpha,H(x_1)\cdots H(x_n),$$
$$(\bar\psi(x')\gamma^\nu)_\beta A_\nu(x')\}|0,0)'_{\text{conn, prop}}dx_1\cdots dx_n$$

and remembering the definition (2·1), we can simply write the expression (2·3) as

$$ie\int S^F(x-y)\gamma^\mu\langle A_\mu(y)\rangle G(yx')\,dy-i\int S^F(x-y)\sum^*(y,y')G(y',x')\,dy\,dy'.$$

Thus (2·2) becomes

$$G(x,x')=iS^F(x-x')+ie\int S^F(x-y)\gamma^\mu\langle A_\mu(y)\rangle G(y,x')\,dy$$
$$-i\int S^F(x-y)\sum^*(y,y')G(y',x')\,dy\,dy'. \qquad (2\cdot5)$$

Therefore the fundamental equation satisfied by G runs[9] to

$$\gamma^\mu(-i\partial_\mu-e\langle A_\mu(x)\rangle)G(x,x')+\int M(x,y)G(y,x')\,dy=\delta(x-x'), \qquad (2\cdot6)$$

where

$$M(x,y)=m\delta(x-y)+\sum^*(x,y),$$

or in the matrix form it may be written as

$$\{\gamma^\mu(P_\mu-e\langle A_\mu\rangle)+M\}G=1\,. \qquad (2\cdot6)'$$

Here the operator $\sum^*$ represents the ordinary proper self-energy as easily seen from its definition (2·4). Particularly suppose that $J_\mu=0$. Then $\langle A_\mu\rangle$ turns to vanish, as will be shown later.

Representing the Green-function, the mass-operator, etc. by $\overset{\circ}{G}$, $\overset{\circ}{M}$,$\cdots$ respectively in this particular case, we have $1/i\,\overset{\circ}{G}=S^F+S^F(-i\overset{\circ}{\sum}{}^*)(1/i\,\overset{\circ}{G})$ instead of (2·5). From the comparison of this equation with Eq. (6·3) of Dyson's paper "The S–matrix in Q. E. D.", it is easily seen that $1/i\,\overset{\circ}{G}$ corresponds to Dyson's S_F'.

We have so far restricted our attention only to $\psi(x)$ in analysing the T–product of G. Conversely, if we analyse G by taking note of $\bar{\psi}$ instead of ψ, we get the alternative forms such as

$$G=iS^F+ieG\gamma^\mu\langle A_\mu\rangle S^F-iG\sum{}^*S^F \tag{2·7}$$

and

$$G\{\gamma^\mu(P_\mu-e\langle A_\mu\rangle)+M\}=1\,. \tag{2·8}$$

From (2·6) and (2·8), we can define the inverse of G unambiguously as

$$G^{-1}=\gamma^\mu(P_\mu-e\langle A_\mu\rangle)+M.$$

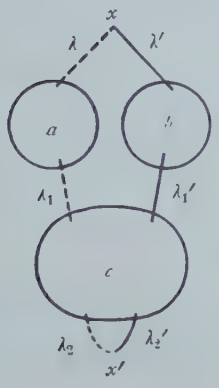

Fig. 4

Finally, let us analyse the operator $\sum{}^*$ defined by (2·4). Consider a graph g_n with $n+2$ vertices corresponding to any one of allowable normal constituents in (2·4), and suppose a photon-line λ_1 and an electron line λ_1', being chosen out of g_n so as to divide n vertices $x_1\cdots x_n$ into three sets a, b, c as in Fig. 4. Then we see that λ_1 is a photon-bridge between a and c and λ' is an electron-bridge between b and c.

The numbers of vertices in a and b change according to the situation that which bridge-lines are chosen out. Here we suppose that the bridge-lines λ_1 and λ_1' are chosen so as to make a and b to be the maximal sets. Then the remaining set c becomes a proper vertex-part defined by Dyson.

Now let us make similar considerations about all the normal constituents arising in (2·4), and carry out seperately the summation over all the contributions from a, b, c. Then $\sum{}^*$ can be written in the following form,

$$\sum{}^*_{\alpha\beta}(xx')=ie^2\gamma^\mu_{\alpha\beta}\int G_{\rho\sigma}(xy)\,\Gamma^\nu_{\sigma\beta}(yx'y')\,\mathfrak{G}_{\nu\mu}(y'x)\,dy\,dy', \tag{2·10}$$

where Γ^ν is the sum of contributions from the set c and is defined by

$$\Gamma^\mu_{\alpha\beta}(xx'\xi)=\gamma^\mu_{\alpha\beta}\delta(x-x')\,\delta(x-\xi)+\Lambda^\mu_{\alpha\beta}(xx'\xi) \tag{2·11}$$

with

$$\Lambda^\mu_{\alpha\beta}(xx'\xi)=-e\sum_{n=1}^{\infty}\frac{(-i)^n}{n\,!}\int(0|T\{A_\nu(x)\,(\gamma^\nu\psi(x))_\alpha,\,(\bar{\psi}(x')\gamma^\lambda)_\beta A_\lambda(x'),j^\mu(\xi),$$

$$H(x_1)\cdots H(x_n)\}|0)'_{\text{conn, prop}}\,dx_1\cdots dx_n\,. \tag{2·12}$$

Here the notation $(|T\{\cdots\}|)'_{\text{conn, prop}}$ has the meaning that in evaluating the T–product, only those terms should be retained which correspond to the proper-vertex parts. The equation (2·10) can be written more compactly as

$$\sum{}^*=ie^2\gamma^\mu G\,\Gamma^\nu\mathfrak{G}_{\nu\mu} \tag{2·10}'$$

by using the matrix notation.

Here we wish to give some remarks about the operators $\sum^*$ and A^μ. In the first place, from the definition of G it holds

$$\frac{\delta G(x,x')}{\delta J_\mu(\xi)} = -\langle \psi(x)\bar{\psi}(x')A_\mu(\xi)\rangle' = B_\mu(xx'\xi).$$

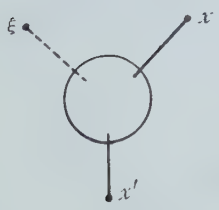

Fig. 5

This quantity can be represented graphically by Fig. 5. If the point ξ' is made to agree with x, Fig. 5 becomes as in Fig. 2. Corresponding to this graphical consideration, we have

$$\lim_{\xi\to x} ie\gamma^\mu \frac{\delta G(xx')}{\delta J_\mu(\xi)} = \sum^* G\,. \tag{2·13}$$

In the second place, let us investigate $\delta\sum^*/\delta J_\mu$. This quantity can be analysed in quite the same way as that used in the analysis of the second term in (2·3). Remembering the definition (2·12), we get the following relation

$$\frac{\delta \sum^*_{\alpha\beta}(xx')}{\delta J_\mu(\xi)} = -e\int \Lambda^\nu_{\alpha\beta}(xx'\xi')\mathfrak{G}_{\nu\mu}(\xi'\xi)d\xi'. \tag{2·14}$$

Therefore, bearing in mind the relation (1·17), (2·9), and the definition (2·11), we obtain the following two relations,

$$\frac{\delta G^{-1}_{\alpha\beta}(xx')}{\delta\langle A_\mu(\xi)\rangle} = -e\,\Gamma^\mu_{\alpha\beta}(xx'\xi), \tag{2·15}$$

$$\frac{\delta \sum^{-1\,*}_{\alpha\beta}(xx')}{\delta\langle A_\mu(\xi)\rangle} = -e\Lambda^\mu_{\alpha\beta}(xx'\xi). \tag{2·14}'$$

Eq. (2·15) can be also directly derived by substituting from (2·10)′ into (2·13). All these equations are just the ones given by Schwinger.

§ 3. Green-function of the one-photon problem

In the first place let us investigate $\langle A_\mu(x)\rangle$. By substituting from (1·11) into (1·13), this quantity may be written as

$$\langle A_\mu(x)\rangle = i\int D^F(x-y)J_\mu(y)dy + i\int D^F(x-y)\langle j_\mu(y)\rangle dy\,, \tag{3·1}$$

or in virtue of the definition of G it runs to

$$\langle A_\mu(x)\rangle = i\int D^F(x-y)[J_\mu(y) + ie\,\mathrm{tr.}\{\gamma^\mu G(yy)\}]dy\,. \tag{3·2}$$

From (3·2) we can easily write down the equation satisfied by $\langle A_\mu\rangle$ in the following form,

$$\Box\langle A_\mu(x)\rangle = -J_\mu(x) - ie\,\mathrm{tr.}\{\gamma^\mu G(xx)\}. \tag{3·3}$$

Suppose now that $J_\mu = 0$. Then $G(xx')$ becomes a function $\overset{\circ}{G}$ of $(x-x')$ having the following simple form owing to its covariant character,

$$\overset{\circ}{G}_{\alpha\beta}(xx') = A((x-x')^2)\,\delta_{\alpha\beta} + \gamma^\mu_{\alpha\beta}(x-x')_\mu B\{(x-x')^2\}, \tag{3·4}$$

where A and B are some invariant functions and may have singularities on the light-cone $(x-x')^2=0$. Assume now $\langle j_\mu(x)\rangle$ to be defined as

$$\langle j_\mu(x)\rangle = ie \lim_{\varepsilon\to 0} \frac{1}{2}[\text{tr.}\{\gamma^\mu G(x, x+\varepsilon)\} + \text{tr.}\{\gamma^\mu G(x, x-\varepsilon)\}].$$

Then, in virtue of (3·4), we have,

$$\langle j_\mu(x)\rangle_{J\to 0} \equiv ie\,\text{tr.}\{\gamma^\mu \mathring{G}(xx)\}=0 \tag{3·5}$$

and

$$\Box\langle \mathring{A}_\mu\rangle = 0\,.$$

From this equation we see that $\langle \mathring{A}_\mu\rangle$ vanishes identically on account of its boundary condition. This fact was already employed in the investigation on the property of $\mathring{G}$ in § 2.

Taking the functional derivative of both sides of (3·3) with regard to $J_\nu(x')$, and remembering the definition of $\mathfrak{G}_{\mu\nu}$, we obtain the following fundamental equation satisfied by $\mathfrak{G}_{\mu\nu}$;

$$\Box\mathfrak{G}_{\mu\nu} = -\delta_{\mu\nu}\delta(x-x') - ie\,\text{tr.}\left\{\gamma_\mu \frac{\delta G(xx)}{\delta J_\nu(x')}\right\}. \tag{3·6}$$

In the second place, let us analyse $\mathfrak{G}_{\mu\nu}$. From (1·16)′, we get

$$\mathfrak{G}_{\mu\nu}(xx') = i\delta_{\mu\nu}D^F(x-x') - \int D^F(x-y)\langle j_\mu(y)A_\nu(x')\rangle' dy$$

by analysing the right-hand side of (1·16)′ in quite the same way as used in case of (2·2). The quantity $\langle j_\mu(y).l_\nu(x)\rangle'$ may be further analysed in more detail following the line of reasoning used in case of Fig. 3. The result thus obtained may be written

$$\mathfrak{G}_{\mu\nu} = i\delta_{\mu\nu}D^F - iD^F P_{\mu\rho}\mathfrak{G}_{\rho\nu} \tag{3·7}$$

with the definition

$$P_{\mu\nu}(xx') = -i\langle j_\mu(x) j_\nu(x')\rangle'_{\text{prop}}\,. \tag{3·8}$$

Here the notation $\langle j_\mu j_\nu\rangle'_{\text{prop}}$ means that in evaluating this quantity, only those contributions should be summed up which arise from the proper photon-self-energy-part.

The integral equation (3·7) gives

$$(\Box\delta_{\mu\rho} - P_{\mu\rho})\mathfrak{G}_{\rho\nu} = -\delta_{\mu\nu} \tag{3·6}′$$

in place of (3·6). From the comparison of (3·6)′ with (3·6), we get the relation

$$P_{\mu\nu} = -ie^2\,\text{tr.}\{\gamma_\mu G\Gamma^\nu \mathfrak{G}_{\nu\mu}\} \tag{3·9}$$

by means of (2·15). (3·9) can be also derived directly by analysing the right-hand side of (3·8) in the same way as in case of Fig. 4. Putting now, $J=0$ in (3·7), we get

$$\left(\frac{1}{i}\mathring{\mathfrak{G}}_{\mu\nu}\right) = \delta_{\mu\nu}D^F - D^F(i\mathring{P}_{\mu\rho})\left(\frac{1}{i}\mathring{\mathfrak{G}}_{\rho\nu}\right).$$

From this expression, we see that $1/i\,\mathring{\mathfrak{G}}_{\mu\nu}$ corresponds to Dyson's D'^F, and $i\mathring{P}_{\mu\rho}$ corresponds to the proper photon-self-energy Π^*.

Next, we shall give some remarks about the Lorentz-condition. The quantity $P_{\mu\nu}$ can be written as

$$P_{\mu\nu}(xx') = ie^2 \,\mathrm{tr.}\{\gamma^\mu S^F(x-x')\gamma^\nu S^F(x'-x)\}$$
$$-ie\int \mathrm{tr.}[S^F(y-x)\gamma^\mu S^F(x-y')\langle e A_\lambda(y')(\gamma^\lambda\psi(y'))\,, e(\bar\psi(y)\gamma^\rho)A_\rho(y)\,, j^\nu(x')\rangle']dydy'. \tag{3·8}'$$

From this expression, we see that

$$\left.\begin{aligned}\frac{\partial P_{\mu\nu}(xx')}{\partial x^\mu}&=0\\ \frac{\partial P_{\mu\nu}(xx')}{\partial x^{\nu'}}&=0\end{aligned}\right\} \tag{3·10}$$

and

bearing in mind the relation

$$\frac{\partial}{\partial y^\mu}\{S^F(x-y)\gamma^\mu S^F(y-x')\}=0\,. \tag{3·11}$$

It must be noted that in proving the relation (3·10) an ambiguity occurs from the first term of (3·8)′. In order to avoid this ambiguity, we assume in this case that

$$-\frac{\partial}{\partial x^\mu}\,\mathrm{tr.}[S^F(x'-x)\gamma^\mu S^F(x-x')\gamma^\nu]$$

is meant by

$$\lim_{\varepsilon\to 0}\frac{\partial}{\partial x^\mu}\,\mathrm{tr.}[S^F(x'-x)\gamma^\mu S^F(x-x'+\varepsilon)\gamma^\nu]$$

instead of

$$\frac{\partial}{\partial x^\mu}\lim_{\varepsilon\to 0}\mathrm{tr.}[S\ (x'-x)\gamma^\mu S^F(x-x'+\varepsilon)\gamma^\nu]\,.$$

Substituting from (3·10) into (3·7) and carrying the integration by parts in the second term of (3·6), we get

$$\frac{\partial \mathfrak{G}_{\mu\nu}(xx')}{\partial x_\mu}=i\frac{\partial D^F(x-x')}{\partial x_\nu}\,, \tag{3·12}$$

provided that the adiabatic assumption on the infinitely remote surfaces σ_1 and σ_1 is taken into account. (3·12) can be also derived from the equation (3·6)′, by taking the four dimensional divergence of it with regard to x_μ and remembering the boundary conditions on σ_1 and σ_2. On the other hand it holds

$$\frac{\partial\langle A_\mu(x)\rangle}{\partial x_\mu}=0 \tag{3·13}$$

by means of the equation

$$\frac{\partial\langle j_\mu(x)\rangle}{\partial x_\mu}=0,\quad\text{and}\quad\frac{\partial J_\mu}{\partial x_\mu}=0\,, \tag{3·14}$$

the first equation in (3·14) being easily verified.

Schwinger has proposed that the expression (3·12) should vanish. We believe he was mistaken in this point.

The relation (3·12) appears at a glance to conflict with the relation (3·13). However, it is easily seen that there is no inconsistencies between (3·12) and (3·13), because of the non-commutability

$$\left[\frac{\delta}{\delta J_\nu(x')}, \frac{\partial}{\partial x_\mu}\right] \neq 0 .^{*)}$$

The results obtained up to the present show that we can give all the quantities and the equations satisfied by them given by Schwinger without use of the curious spinors η and $\bar{\eta}$. The quantities M, $\Gamma'_{\mu\nu}$, and Γ''^{ν} turned to be understood as the proper self-energy of an electron, a photon and the proper vertex-part respectively.

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*) $$\frac{\partial}{\partial x_\mu}\left(\frac{\delta\langle A_\mu[x;J]\rangle}{\delta J_\nu(x')}\right)=\lim_{\Delta J\to 0}\frac{1}{\Delta J}\left[\frac{\partial}{\partial x_\mu}\langle A_\mu[x;J+\Delta J]\rangle-\frac{\partial}{\partial x_\mu}\langle A_\mu[x;J]\rangle\right].$$

On account of (3·13) this turns into

$$\lim_{\Delta J\to 0}\frac{1}{\Delta J}\left[\frac{\partial}{\partial x_\mu}\langle A_\mu[x;J+\Delta J]\rangle\right].$$

Using (3·1), we get

$$\frac{\partial}{\partial x_\mu}\left(\frac{\delta\langle A_\mu[x;J]\rangle}{\delta J_\nu(x')}\right)=i\lim_{\Delta J\to 0}\frac{1}{\Delta J}\int D^F(x-y)\frac{\partial}{\partial y_\mu}(J_\mu(y)+\Delta J_\mu(y))dy$$

$$+i\lim_{\Delta J\to 0}\frac{1}{\Delta J}\int D^F(x-y)\frac{\partial}{\partial y_\mu}\langle j_\mu[y;J+\Delta J]\rangle dy .$$

By means of (2·6) we can verify

$$\frac{\partial}{\partial y_\mu}\langle j_\mu[y;J+\Delta J]\rangle=0 .$$

Hence

$$\frac{\partial \mathfrak{G}_{\mu\nu}}{\partial x_\mu}\equiv\frac{\partial}{\partial x_\mu}\left(\frac{\delta\langle A_\mu[x;J]\rangle}{\delta J_\nu(x')}\right)=i\frac{\partial D^F(x-x')}{\partial x_\mu}.$$

On the other hand, we have

$$\frac{\delta}{\delta J_\nu(x')}\left(\frac{\partial A_\mu[x;J]}{\partial x_\mu}\right)=0 .$$

Thus we see in general

$$\left[\frac{\partial}{\partial x_\mu}, \frac{\delta}{\delta J_\nu(x')}\right]\langle A_\mu[x;J]\rangle=i\frac{\partial D^F(x-x')}{\partial x_\mu}.$$

However, only in the special case, where

$$\frac{\partial \Delta J_\nu(x')}{\partial x_\nu'}=0 ,$$

we get

$$\frac{\partial}{\partial x_\mu}\left(\frac{\delta\langle A_\mu[x;J]\rangle}{\delta J_\nu(x')}\right)=0 .$$

The variation ΔJ_ν considered in (1·17) does not satisfy the restriction

$$\frac{\partial \Delta J_\nu}{\partial x_\nu}=0 .$$

This is obvious because of (3·12).

The authors wish to thank Prof. S. Tomonaga for his valuable discussion about this problem.

Finally some remarks will be given about the rule for obtaining the Green-function of the many-body problem. Suppose a transition process from an initial state where m-positrons and n electrons are incident, to a final state in which m' positrons and n' electrons are outgoing. The Green-function G corresponding to this process is given by

$$G(x_1\cdots x_N x_1'\cdots x_{N'}')=\text{const.}\langle\psi(x_1)\cdots\psi(x_N)\bar{\psi}(x_1')\cdots\bar{\psi}(x_{N'}')\rangle$$

with $$N=n+m'=n'+m$$

where the multiplying constant may be properly chosen.

If there are p photons moreover in the initial state, and q photons in the final state, then the Green-function, in this case, may be obtained in the following way;

$$\frac{\partial^M G(x_1\cdots x_N x_1'\cdots x_{N'}')}{\partial f_{\mu_1}(\xi_1)\cdots\partial f_{\mu_M}(\xi_M)},$$

where

$$M=p+q.$$

§ 4. Removal of divergences arising in several quantities

In order to remove divergences arising in the several quantities G, M, $\mathfrak{G}$ etc. we shall follow the line of reasoning of Dyson and Gupta. The Lagrangian density proposed by them may be written as

$$L^*=-\frac{1}{4}F_{\mu\nu}^*F_{\mu\nu}^*-\frac{1}{2}\left(\frac{\partial A_\mu^*}{\partial x_\mu}\right)^2-\bar{\psi}(-i\gamma^\mu\partial_\mu+m)\psi+\delta m\bar{\psi}\psi+A_\mu^*(J_\mu^*+e\bar{\psi}\gamma_\mu\psi), \tag{4·1}$$

where any stared quantity represents the unrenormalized one, and the quantities without the asterisk represent the renormalized ones which are physically observable. The physically observable potential A_μ is defined by

$$A_\mu=\theta A_\mu^* \quad \theta=e/e_1, \tag{4·2}$$

where e is the unrenormalized electronic charge and e_1 the renormalized charge. Similarly, the renormalized external current J_μ is defined by

$$J_\mu=\theta^{-1}J_\mu^*. \tag{4·3}$$

(Strictly speaking, A_μ, e_1 and J_μ are not yet free of divergences. To remove the remaining divergences it is further necessary to perform the transformation (4·13).)

The Lagrangian density represented in terms of renormalized quantities is

$$L=-\frac{1}{4}F_{\mu\nu}F_{\mu\nu}-\bar{\psi}(-i\gamma^\mu\partial_\mu+m)\psi-\frac{1}{2}\left(\frac{\partial A_\mu}{\partial x_\mu}\right)^2+(J_\mu+j_\mu)A_\mu+\delta m\bar{\psi}\psi+\frac{f}{4}F_{\mu\nu}F_{\mu\nu}, \tag{4·4}$$

where f and j_μ are given by

$$f=1-\theta^2 \quad \text{and} \quad j_\mu=\frac{e_1}{2}\{\bar{\psi}\gamma_\mu\psi-\gamma_\mu\psi\cdot\bar{\psi}\},$$

It must be noted that L is not exactly equal to L^* expressed in terms of the renormalized quantities. About the latter Lagrangian some remarks will be given in the appendix.

The Hamiltonian density in the Tomonaga-Schwinger representation corresponding to the Lagrangian (4·4) is

$$H=-\frac{f}{4}F_{kl}F_{kl}-\frac{f'}{2}F_{k4}^2-\delta m\bar{\psi}\psi-A_\mu(J_\mu+j_\mu),\quad f'=f/(1-f), \tag{4·5}$$

where the Greek subscripts assume values ranging from 1 to 4, whereas the Latin ones from 1 to 3.

Substituting this Hamiltonian into the definition of G, and performing the same analysis as that of § 2 we obtain the following relation

$$G=iS^F+ie_1S^F\gamma^\mu\langle A_\mu\rangle G-iS^F\sum{}^*G+i\delta mS^FG\,, \tag{4·6}$$

where $\langle A_\mu\rangle$, $\sum^*$ are similarly defined as in case of § 2.

From (4·6), we get the equation

$$[\gamma_\mu(p_\mu-e_1\langle A_\mu\rangle)+m+\sum{}^*-\delta m]G=1\,. \tag{4·7}$$

The following several relations can be also derived,

$$\lim_{\xi\to x}ie_1\gamma^\mu\frac{\delta G(xx')}{\delta J_\mu(\xi)}=\int\sum{}^*(xy)\,G(yx')\,dy, \tag{4·8}_a$$

$$\frac{\delta G^{-1}(xx')}{\delta\langle A_\mu(\xi)\rangle}=-e_1\Gamma^\mu(xx'\xi), \tag{4·8}_b$$

$$\frac{\delta\sum^*}{\delta\langle A_\mu\rangle}=-e_1A^\mu, \tag{4·8}_c$$

$$\sum{}^*=ie_1^2\gamma^\mu G\Gamma^\nu\mathfrak{G}_{\nu\mu}, \tag{4·8}_d$$

$$\mathfrak{G}_{\mu\nu}(xx')=\frac{\delta\langle A_\mu(x)\rangle}{\delta J_\nu}\,. \tag{4·8}_e$$

In this case the fundamental equations satisfied by $\langle A\rangle$ and $\mathfrak{G}$ are written as

$$\left\{\Box\delta_{\mu\nu}+f\left(\frac{\partial^2}{\partial x_\mu\partial x_\nu}-\Box\delta_{\mu\nu}\right)\right\}\langle A_\nu\rangle=-\{J_\mu+ie_1\,\mathrm{tr.}\,(\gamma_\mu G)\} \tag{4·9}$$

and

$$\{\Box\delta_{\mu\rho}-L_{\mu\rho}\}\,\mathfrak{G}_{\rho\nu}=-\delta_{\mu\nu}\cdot1 \tag{4·10}$$

with the definition

$$\left.\begin{aligned}L_{\mu\rho}&=P_{\mu\rho}+f(\delta_{\mu\rho}\Box-\partial^2/\partial x_\mu\partial x_\rho),\\P_{\mu\rho}&=-ie_1^2\,\mathrm{tr.}\,(\gamma^\mu G\Gamma^\nu G).\end{aligned}\right\} \tag{4·11}$$

The polarization operator $P_{\mu\nu}$ satisfies also in this case, the identities

$$\frac{\partial P_{\mu\nu}}{\partial x_\mu}=\frac{\partial P_{\mu\nu}}{\partial x_\nu'}=0\,. \tag{4·12}$$

Here it is remarked that in deriving the equations (4·9) and (4·10) there occur some new complications owing to the time-derivative appearing in H. The interested reader is recommended to refer to the appendix where the similar situation will occur.

As already noted, the several quantities introduced here are not yet free from divergences. To complete the removal of divergences let us perform the following transformation :

$$\left.\begin{aligned} &G'=a^{-1}G, \quad c_1'=\sqrt{a}\,c_1, \quad c'=\sqrt{a}\,c, \quad J'=\frac{1}{\sqrt{a}}J, \\ &\langle A\rangle'=\frac{1}{\sqrt{a}}\langle A\rangle, \quad \mathfrak{S}'=\mathfrak{S}, \quad P'=P, \\ &I''=aI', \quad \Lambda'=a\Lambda, \quad \sum^{*\prime}=a\sum^{*}, \\ &f'=1-\left(\frac{c_1'}{c'}\right)^2=f, \end{aligned}\right\} \tag{4·13}$$

where a is an yet undetermined constant, being a function of c_1'. Corresponding to this transformation, the equations (4·7)–(4·12) turn into

$$[\gamma^\mu p_\mu+m+K']G'=1, \tag{4·14}$$

$$[\Box\delta_{\mu\rho}-L'_{\mu\rho}]\mathfrak{S}'_{\rho\nu}=-\delta_{\mu\nu}\cdot 1, \tag{4·15}$$

$$\left[\Box\delta_{\mu\nu}+f'\left(\frac{\partial^2}{\partial x_\mu\partial x_\nu}-\Box\delta_{\mu\nu}\right)\right]\langle A_\nu\rangle'=-\{J_\mu'+ic_1'\,\mathrm{tr.}\,(\gamma_\mu G')\}, \tag{4·16}$$

$$\frac{\delta\langle A_\mu\rangle'}{\delta J_\nu'}=\mathfrak{S}'_{\mu\nu}, \tag{4·17}$$

where

$$K'=(a-1)(\gamma^\mu p_\mu+m)-ac_1'\gamma^\mu\langle A_\mu\rangle'+\sum^{*\prime}-a\delta m, \tag{4·18}$$

$$L'_{\mu\nu}=P'_{\mu\nu}+f'\left(\delta_{\mu\nu}\Box-\frac{\partial^2}{\partial x_\mu\partial x_\nu}\right) \tag{4·19}$$

and

$$\sum^{*\prime}=ic_1'^2\gamma^\mu G'\Gamma^{\mu\prime}\mathfrak{S}'_{\nu\mu}, \tag{4·20}$$

$$P'_{\mu\nu}=ic_1'^2\,\mathrm{tr.}\,(\gamma_\mu G'\Gamma'_\nu G'), \tag{4·21}$$

$$\frac{\delta\sum^{*\prime}}{\delta\langle A_\mu\rangle'}=-c_1'\Lambda'^\mu, \tag{4·22}$$

$$\Gamma^{\mu\prime}=a\gamma^\mu+\Lambda^{\mu\prime}=\gamma^\mu+\{\Lambda^{\mu\prime}+(a-1)\gamma^\mu\}. \tag{4·23}$$

Note that all these new equations have just the same forms as those in (4·7)–(4·12) except (4·18) and (4·23). This fact allows us to make use of Dyson's conclusions concerning the primitive divergences.

Let us prove that all the primed quantities now introduced are free of divergences and can be understood as being physically observable directly or indirectly. Unfortunately, we can not show the above mentioned assertion without use of the assumption that the infinite series in powers of c_1' is convergent whenever it appears. This assumption will be supposed in the following pages as in the theory of S-matrix. From (4·14), G' may be written as

$$G'=i\sum_{n=0}^{\infty}(-i)^n(S^FK')^nS^F. \tag{4·24}$$

In order to show G' being free from divergences, it is only necessary to prove the finiteness of each term in (4·24) by virtue of the assumption stated above. The n-th term in (4·24) runs to

$$(-i)^{n-1}(k|(S^F K')^n S^F|k') = (-i)^{n-1}\int S^F(k)K'(kk_1)S^F(k_1)K'(k_1k_2)\cdots K'(k_{n-1}k')S^F(k')\,dk_1\cdots dk_{n-1} \tag{4·25}$$

in the momentum space, where K' has the following form;

$$K'(kk') = \sum_{j=0}^{\infty}\int K_j''(kp_1\cdots p_j)J'(p_1)J'(p_2)\cdots J'(p_j)\,\delta(k+\sum p_i-k')\,dp_1\cdots dp_j\,. \tag{4·26}$$

Here $J'(p)$ is the Fourier-coefficient of $J_\mu'(x)$ and δ-factor results from the conservation of energy and momentum. Suppose now that $K'(kk')$ is free from divergences, then the contributions from the terms with $j\geq 1$ in (4·24) to the intergral (4·25) can be made not to give rise to any divergences provided that the external current is properly chosen. That is to say, the external current is supposed to be chosen in such a way that the amplitude $J'(p)$ decreases so rapidly enough as to make the integral in consideration converge. On the other hand the term with $j=0$ in (4·26) does not contain $J(p)$, however, since this term has the factor $\delta(k-k')$, there occurs no divergence in (4·25).

These considerations are sufficient to show that the proof of finiteness of K' is only necessary for our purpose. The same is true in case of $\mathfrak{G}'$. That is, it is only necessary in case of $\mathfrak{G}'$ to prove the finiteness of $L_{\mu\nu}'$.

Suppose now that the quantities G', $\mathfrak{G}'$, K', etc. are expanded into series in powers of e_1', the coefficients of which are G_n' $\mathfrak{G}_n'\cdots\cdots(n=0,1,2,\cdots)$. Then our task is to prove the finiteness of these coefficients for any arbitrary n by using the mathematical induction. Speaking in more detail, under the assumption that all the coefficients G_j' $\mathfrak{G}_j'\cdots$with $j\leq n-1$ are free from divergences, we shall prove the finiteness of G_n' $\mathfrak{G}_n'\cdots$for an arbitrarily chosen n. The proof will be given by using the momentum representation.

1) *Finiteness of* $L_{\mu\nu}'$

From (4·21), it is easily seen that $(P_{\mu\nu}')_n$ is a sum of matrix products of G_j', Γ_k' with $j\leq n-2$, $k\leq n-2$. Thus the internal divergences do not appear in $(P')_n$ on account of the assumption stated above. Now $(P')_n$ can be written as

$$(k|P_n'|k') = \delta(k-k')\mathring{P}_n'(k) + (k|P_{nF}'|k') \quad n\geq 2\,,$$

where the first term is independent on $J(p)$ whereas the second is a power series in J, the lowest order of which is the second by means of Furry's theorem. Therefore any term of the series P_{nF}' contains at least four external photon lines. Hence all these terms are finite because of the Dyson's criterion of the primitive divergence. Here it must be noted that G', $\mathfrak{G}'$ and Γ' correspond to Dyson's S_{F_1}', D_{F_1}' and Γ_{μ_1}' respectively. This important fact, which allows us to apply Dyson's criterion to our case, results from the situation that the system of equations (4·14)–(4·23) has the same expressions as those of (4·7)–

(4·12) with the exception of (4·18) and (4·23), and the unprimed quantities G, $\mathfrak{S}$ and I' are easily understood as corresponding to Dyson's S_F' D_F' and Γ' except some modifications by means of the graphical consideration. We can directly ascertain this fact by solving successively the equations (4·14)–(4·23).

The factor $\mathring{P}_n'(k)$ in the first term has the following form

$$(\mathring{P}_{\mu\nu}'(k))_n = A_n(\delta_{\mu\nu}k^2 - k_\mu k_\nu) + \mathring{P}_{\mu\nu}'(k)_{n,f}, \quad (n \geq 2)$$

on account of its covariant character and the identities

$$\frac{\partial P_{\mu\nu}'(xx')}{\partial x_\mu} = \frac{\partial P_{\mu\nu}'(xx')}{\partial x_\nu'} = 0 .$$

Here A_n is a constant and diverges never more strongly than as a power of a logarithm and the second term is finite.

Suppose now that f' is defined by

$$f' \equiv f'(e_1') = \sum_{n=2}^{\infty} e_1'^n A_n = Z_3(e_1') .$$

Then L_n' turns into

$$e_1'^n(k|L_{\mu\nu}'|k')_n = e_1'^n[\{A_n(\delta_{\mu\nu}k^2 - k_\mu k_\nu) + \mathring{I}_{\mu\nu}'(k)_{n,f}\}\delta(k-k') + (k|P_{\mu\nu F}'|k')_n] - \delta(k-k')e_1'^n A_n(\delta_{\mu\nu}k^2 - k_\mu k_\nu)$$

which is finite. Accordingly, the finiteness of $\mathfrak{S}_n'$ is proved on account of the remarks stated in page 21.

2) *Finiteness of* $\langle A_\mu \rangle'$

Consider the expansion of $\mathfrak{S}'$ in powers of J', which is given by

$$\mathfrak{S}' = \mathring{\mathfrak{S}}' + \int \frac{\delta \mathfrak{S}'}{\delta J'(\xi)}\Big)_{J'=0} J'(\xi)\,d\xi + \frac{1}{2!}\int \frac{\delta^2 \mathfrak{S}'}{\delta J'(\xi)\,\delta J'(\xi')}\Big)_{J'=0} J'(\xi)J'(\xi')\,d\xi\,d\xi' + \cdots .$$

Solving the system of equations (4·14)–(4·23) by using the power expansion in e_1' and J', we see that

$$\frac{\delta^{2n+1}\mathfrak{S}'}{\delta J'^{2n+1}}\Big)_{J'=0} = 0 \quad \text{and} \quad \frac{\delta^{2n}\mathfrak{S}'}{\delta J'^{2n}}\Big)_{J'=0} = e_1'^{2n+2}B_n \quad (n=1, 2\cdots)$$

hold, where the first equation is derived from the Furry's theorem. The quantity B_n in the second equation has the following expression

$$B_n = \sum_{n=0}^{\infty} e_1'^k B_{n,k} \quad \text{with} \quad B_{n,0} \neq 0 \qquad (n=0, 1, 2\cdots)$$

where B_{nk} does not explicitly involve e_1' but is a functional of $\mathring{G}'$, $\mathring{\mathfrak{S}}'$ and $\mathring{I}''$. Accordingly, it can be also expanded in powers of e_1', that is,

$$B_{n,k} = \sum_{l=0}^{\infty} e_1'^l B_{n,k,l} .$$

The coefficient B_{nkl} is a sum of products of $\mathring{G}_i'$ $\mathring{\mathfrak{S}}_i'$ and $\mathring{I}_i''$ with $i \leq l$.

By using (4·24) and (4·17), $\langle A \rangle'$ may be written as

$$\langle A\rangle' = \int \mathring{\mathfrak{G}}'(x\xi) J'(\xi) d\xi + \sum_{k=1}^{\infty} \frac{(e_1')^{2k+2}}{(2k+1)!} \int B_k(x\xi\xi,\cdots\xi_{2k}) \times J'(\xi) J'(\xi_1)\cdots J'(\xi_{2k}) d\xi\, d\xi_1 \cdots d\xi_{2k}.$$

Therefore we get

$$\langle A\rangle_n' = \int \mathring{\mathfrak{G}}_n J'(\xi) d\xi + \sum_{\substack{k=1 \\ (2k+2+j=n)}}^{\leq \frac{n-2}{2}} \frac{1}{(2k+1)!} \int C_{k,j} J'(\xi) J'(\xi_1)\cdots J'(\xi_{2k}) d\xi\, d\xi_1 \cdots d\xi_{2k}, \tag{4·27}$$

where C_{kj} is given by

$$C_{kj} = \sum_{\substack{kl \\ (h+l=j)}} B_{khl}.$$

Since the second term contains $\mathring{G}_i' \mathring{\mathfrak{G}}_i'$ and $\mathring{\Gamma}_i'$ with $i \leq n-4$ on account of the definition of C_{kj} and $B_{n,k,l}$, it does not involve any internal divergence according to Dyson's criterion. The finiteness of the first term in (4·27) is already proved. Thus $\langle A\rangle_n'$ is finite.

3) *Finiteness of K'*

Following the line of reasoning used in case of $L_{\mu\nu}'$, we expand $\sum^{*\prime}$ in powers of $\langle A\rangle'$ in the following way,

$$\sum^{*\prime} = \mathring{\sum}^{*\prime} - e_1' \mathring{\Lambda}' \langle A\rangle' + \sum_F^{*\prime},$$

where $\sum_F^{*\prime}$ is a power series in $\langle A\rangle'$, beginning at the second order of it, each coefficient of which is a functional of $\mathring{G}'$ $\mathring{\Gamma}'$ and $\mathring{\mathfrak{G}}'$. Accordingly $\sum_{Fn}^{*\prime}$ is finite on account of the Dyson's criterion and the finiteness of $\langle A\rangle'$ just proved.

The n-th coefficient in the expansion of $\mathring{\sum}^{*\prime}$ in terms of e_1' has the following form

$$\begin{aligned}(k|\mathring{\sum}_n^{*\prime}|k') &= \delta(k-k')\,\mathring{\sum}^{*\prime}(k) \\ &= \delta(k-k')[A_n' + B_n(k_\mu \gamma^\mu + m) + \mathring{\sum}_{fn}^{*\prime}(k)] \quad n \geq 2 \end{aligned} \tag{4·28}$$

in the momentum representation. Here the constant A_n' diverges at most linearly, and the constant B_n at most logarithmically, and the remaining part $\mathring{\sum}_{fn}^{*\prime}$ is finite.

Similarly, on account of the covariant character of $\mathring{\Lambda}^{\mu\prime}$, it can be written as

$$(k|\mathring{\Lambda}_n^{\mu\prime}|k') = \gamma_\mu L_n + \mathring{\Lambda}_{f,n}^{\mu}(kk') \quad n \geq 2, \tag{4·29}$$

where L_n is a constant diverging at most logarithmically, and $\mathring{\Lambda}_{f,n}^{\mu}$ is finite.

Substituting these expressions into (4·18), we get

$$\begin{aligned}(k|K_n'|k') &= \delta(k-k')[\{A_n' - (a\delta m)_n\} + (a-1+B)_n(k_\mu\gamma^\mu + m)] \\ &\quad - \sum_{j=0}^{n-1} (a-1+L)_{n-j-1} \gamma^\mu (k|\langle A_\mu\rangle_j'|k') + \delta(k-k')\,\mathring{\sum}_{fn}^{*\prime}(k) + \sum_{nF}^{*\prime}(kk') \\ &\quad - \sum_{j=0}^{n-1} \{\gamma^\mu + \mathring{\Lambda}_f^\mu(kk')\}_{n-j-1} (k|\langle A_\mu\rangle_j'|k'), \quad (n \geq 2),\end{aligned}$$

where $\{\ \}_n$ represent the n-th coefficient of the expansion of $\{\ \}$ in terms of e_1'.

Suppose now that the unknown parameter a is chosen in the following way;

$$a=1-\sum_{n=2}^{\infty} B_n e_1'^n=Z_2(e_1') \tag{4·30}$$

and further δm is determined by

$$a\delta m=\sum_{n=2}^{\infty} A_n' e_1'^n . \tag{4·30}'$$

Then K_n' turns to finite by means of the finiteness of $\langle A\rangle'$ and the following important relation

$$L_n=B_n$$

which will be proved in the next section.

4) *Finiteness of* Γ'^{μ}

Γ'^{μ} may be divided into two parts, such as

$$\Gamma_n'^{\mu}=\mathring{\Gamma}_n'^{\mu}+\Gamma_{nF}'^{\mu},$$

where the first term does not contain J''s and the second term is a series in powers of J', beginning at the first order of it. Following the line of the same reasoning as in the preceding cases, we can show the second term being free of divergences. From (4·23) and (4·29) we have

$$\begin{aligned}\mathring{\Gamma}_n'^{\mu}(kk'l)&=\delta(k-k'+l)\{a_n\gamma^{\mu}+(k|\mathring{A}_n'^{\mu}|k')\}\\&=[\{L_n+(a-1)_n\}\gamma^{\mu}+\mathring{A}_{nf}'^{\mu}(kk')]\delta(k-k'+l),\quad n\leq 2 .\end{aligned}$$

Therefore $\Gamma_n'^{\mu}$ is finite on account of (4·30).

Thus, the proof of the finiteness of $\mathfrak{S}'$, $\langle A\rangle'$, G' and Γ' is completed under the assumption stated in page 20. The present theory seems quite satisfactory because of the fact that several quantities appearing in the system of equations (4·14)–(4·23) are free from divergences, accordingly, the internal divergences are explicitly eliminated in evaluating $\sum'^{*}$ and $P_{\mu\nu}'$.

In concluding this section we shall give a short remark about f'. f' is defined by

$$f'=1-\frac{e_1'^2}{e'^2}\equiv\varphi'(e_1')=1-\frac{e_1^2}{e^2}=f=\varphi(e) .$$

Putting

$$e=g(e_1'),$$

we have

$$\varphi(e)=\varphi[g(e_1')]\equiv\varphi'(e_1').$$

Therefore the function φ has not the same form as that of φ'. Since in the present paper φ' is determined by

$$\varphi'(e_1')=Z_3(e_1'),$$

$\varphi(e)$ is not equal to $Z_3(e)$. Accordingly the divergence of the unprimed polarization operator $P_{\mu\nu}$ can not be cancelled out by its counter term.

§ 5. Gauge transformation and Ward's identity[8]

In this section we shall investigate the covariant character of the several quantities under the gauge transformation.

Since the present theory is based upon the gauge-invariant theory of Tomonaga and Schwinger, the systems of equations (4·7–4·12) must be invariant under the gauge transformation.

Now the unprimed Green-function G may be written in the Heisenberg representation as

$$G(xx')=i(\Psi^*_{\text{vac}},\ ST(\boldsymbol{\phi}(x),\ \bar{\boldsymbol{\phi}}(x'))\Psi_{\text{vac}}),$$

where the heavy type is used for operators in Heisenberg representation. Consider the gauge transformation ;

$$\left.\begin{aligned}&\boldsymbol{\phi}\to\boldsymbol{\phi}=e^{ie_1\lambda}\boldsymbol{\phi},\\&\bar{\boldsymbol{\phi}}\to\bar{\boldsymbol{\phi}}=e^{-ie_1\lambda}\bar{\boldsymbol{\phi}},\\&\boldsymbol{A}_\mu\to\boldsymbol{A}_\mu=\boldsymbol{A}_\mu+\frac{\partial\lambda}{\partial x_\mu}.\end{aligned}\right\}\qquad(5\cdot1)$$

Then G is transformed into

$$G(xx')=e^{ie_1\lambda(x)}\,G(xx')\,e^{-ie_1\lambda(x')}\qquad(5\cdot2)$$

owing to the fact that S is invariant under the boundary condition

$$\lim_{x_0\to\pm\infty}\lambda(x)=0\,.$$

Substituting from (5·2) into (4·7), we get

$$G^{-1}=\gamma^\mu p_\mu+m+K\to\underline{G}^{-1}=e^{ie_1\lambda(x)}\,G^{-1}e^{-ie_1\lambda(x')}\qquad(5\cdot3)$$

by virtue of the gauge covariant character of (4·7).

Writing (5·3) explicitly, as follows,

$$\begin{aligned}&m+\gamma^\mu p_\mu+\{-e_1\gamma^\mu\langle A_\mu\rangle+\sum\nolimits^*-\delta m\}\\&\quad=\gamma^\mu e^{ie_1\lambda(x)}\,p_\mu\,e^{-ie_1\lambda(x')}+m+e^{ie_1\lambda(x)}\{-e_1\gamma^\mu\langle A_\mu\rangle+\sum\nolimits^*-\delta m\}\,e^{-ie_1\lambda(x')},\end{aligned}$$

we obtain the transformation-rules of $\sum^*$ and $\langle A\rangle$, which are given by

$$\left.\begin{aligned}&\langle\underline{A}_\mu\rangle=\langle A_\mu\rangle+\frac{\partial\lambda}{\partial x_\mu},\\&\underline{\sum}^*(xx')=e^{ie_1\lambda(x)}\sum^*(xx')\,e^{-ie_1\lambda(x')}.\end{aligned}\right\}\qquad(5\cdot4)$$

From (5·4) and $(4\cdot8)_e$, we see that $\mathfrak{G}$ is gauge invariant, namely,

$$\mathfrak{G}_{\mu\nu}=\frac{\delta\langle A_\mu\rangle}{\delta J_\nu}=\frac{\delta\langle A_\mu\rangle}{\delta\underline{J}_\nu}=\mathfrak{G}_{\mu\nu}\,.\qquad(5\cdot5)$$

Since (4·10) is gauge invariant, we get

$$\underline{P}_{\mu\nu}=P_{\mu\nu}=\text{invariant}\qquad(5\cdot6)$$

from (5·5) and (4·10). Substituting (5·2) into (5·6) and remembering the relation (4·11), we get

$$\Gamma^{\mu}(xx'\xi)=e^{ie_1\lambda(x)}\,\Gamma^{\mu}(xx'\xi)\,e^{-ie_1\lambda(x')}, \tag{5·7}$$

similarly

$$A^{\mu}(xx'\xi)=e^{ie_1\lambda(x)}\,A^{\mu}(xx'\xi)\,e^{-ie_1\lambda(x')}. \tag{5·8}$$

Conversely, we can easily verify the covariance of the equations (4·7)–(4·12) by using the relations (5·2)–(5·8) here obtained.

Now let us prove the important relation, such as

$$i(\lambda(x)-\lambda(x'))\sum^{*}(xx')=-\int A^{\mu}(xx'\xi)\frac{\partial\lambda(\xi)}{\partial\xi^{\mu}}d\xi\,. \tag{5·9}$$

Suppose that $\lambda(x)$ is infinitesimal. Then from the definition (2·4), we have

$$\begin{aligned}
\delta\sum^{*}(xx') &\equiv \sum^{*}-\sum^{\prime *}\\
&=-ie_1^{2}\sum_{0}^{\infty}\frac{(-i)^n}{n!}\int(0|T\left\{\frac{\partial\lambda(x)}{\partial x_{\mu}}\gamma^{\mu}\psi(x),\ \bar{\psi}(x')\gamma A(x'),\right.\\
&\qquad \left.H(x_1)\cdots H(x_n)\right\}|0)'_{\text{conn, prop}}\,dx_1\cdots dx_n\\
&\quad -ie_1^{2}\sum_{0}^{\infty}\frac{(-i)^n}{n!}\int(0|T\left\{A(x)\gamma\psi(x),\ \bar{\psi}(x')\gamma_{\mu}\frac{\partial\lambda(x')}{\partial x_{\mu}'},\right.\\
&\qquad \left.H(x_1)\cdots H(x_n)\right\}|0)'_{\text{conn, prop}}\,dx_1\cdots dx_n\\
&\quad +e_1^{2}\sum_{0}^{\infty}\frac{(-i)^n}{n!}\int(0|T\{A\gamma\psi(x),\ \bar{\psi}\gamma A(x'),\ j_{\mu}(\xi),\\
&\qquad H(x_1)\cdots H(x_n)\}|0)'_{\text{conn, prop}}\frac{\partial\lambda(\xi)}{\partial\xi_{\mu}}d\xi\,dx_1\cdots dx_n\,,
\end{aligned} \tag{5·10}$$

where the first and second terms result from the variation of $A(x)$ and $A(x')$ in $\sum^{\prime *}(xx')$ respectively, whereas the last term from that of $A(\xi)$ contained in $H(\xi)$. Now in the expansion of the expression

$$(0|T\{\psi(x),\ \bar{\psi}(x')\gamma A(x'),\ H(x_1)\cdots H(x_n)\}|0)'_{\text{conn}}$$

into the sum of normal constituents, there are no terms which correspond to proper diagrams owing to the operator $\psi(x)$. Thus the first term in (5·10) vanishes. The same is true in case of the second term. The remaining term turns to

$$-e_1\int A^{\mu}(xx'\xi)\frac{\partial\lambda(\xi)}{\partial\xi_{\mu}}d\xi$$

by means of the definition (2·12). Thus the proof of (5·9) is completed.

Put $J=0$ in (5·9) and represent it in the momentum space, then (5·9) turns to

$$\lambda(k-k')\{\mathring{\sum}^{*}(k)-\mathring{\sum}^{\prime *}(k')\}=\lambda(k-k')\,\mathring{A}^{\mu}(kk')\,(k-k')_{\mu}\,,$$

bearing in mind that $\mathring{\sum}^{*}(xx')$ is a function of $(x-x')$ and $\mathring{A}^{\mu}(xx'\xi)$ a function of $(x-\xi)$ and $(x'-\xi)$. Since $\lambda(x)$ satisfies the wave equation

$$\Box\lambda=0\,,$$

$(k-k')$ in the above equation must be a null-vector. Suppose now that $(k-k')_\mu=\varepsilon_\mu$ is chosen to be $(\varepsilon, 0, 0, \pm\varepsilon)$ and ε is infinitesimal. Then the above equation becomes

$$\frac{\partial\mathring{\Sigma}^*(k)}{\partial k_\mu}\varepsilon_\mu=\left(\frac{\partial\mathring{\Sigma}^*(k)}{\partial k_1}\pm\frac{\partial\mathring{\Sigma}^*(k)}{\partial k_0}\right)\cdot\varepsilon$$
$$=\mathring{\Lambda}^\mu(k,k)\varepsilon_\mu=\varepsilon\mathring{\Lambda}^1(k,k)\pm\mathring{\Lambda}^0(k,k))\,.$$

From this relation, we get

$$\frac{\partial\mathring{\Sigma}^*(k)}{\partial k_\mu}=\mathring{\Lambda}^\mu(k,k),\quad(\mu=1,2,3,0).\tag{5·10}$$

It will be easily seen that the similar relation also holds between $\mathring{\Sigma}'^*$ and $\mathring{\Lambda}'^\mu$, viz.,

$$\frac{\partial\mathring{\Sigma}^{*\prime}(k)}{\partial k_\mu}=\mathring{\Lambda}^{\mu\prime}(k,k).\tag{5·10}'$$

Substituting from (4·28) and (4·29) into (5·10)′, we obtain

$$L_n=B_n\,.$$

Therefore we get the Ward's identity, namely,

$$Z_1(e_1')=1-\sum_2^\infty L_n e_1'^n=1-\sum_2^\infty B_n e_1'^n=Z_2(e_1')\,.$$

This identity played an important role, as we have already seen, in the proof of removability of divergences.

Now let us investigate the transformation character of any quantity $\langle F\rangle$ under the infinitesimal gauge transformation. The variation of $\langle F\rangle$ may be written as

$$\delta\langle F\rangle=\langle F\rangle-\langle F\rangle$$
$$=\langle\delta F\rangle+i\sum_{n=0}^\infty\frac{(-i)^n}{n!}\int(0|T\{F,j_\mu(\xi),H(x_1)\cdots H(x_n)\}|0)'_{\text{conn}}\frac{\partial\lambda(\xi)}{\partial\xi^\mu}\,d\xi\,dx_1\cdots dx_n\,,\tag{5·11}$$

where the second term results from the variation of A_μ involved in the Hamiltonian, whereas the first one results from the variation of F itself. The second term may be simply written as

$$i\int\langle F,j_\mu(\xi)\rangle'\frac{\partial\lambda(\xi)}{\partial\xi_\mu}d\xi\,.$$

Since the relation

$$i\langle F,j_\mu(\xi)\rangle'=-\frac{\delta\langle F\rangle}{\delta\langle A_\mu(\xi)\rangle}$$

may be easily verified, (5·11) becomes

$$\delta\langle F\rangle=\int\frac{\delta\langle F\rangle}{\delta\langle A_\mu(\xi)\rangle}\frac{\partial\lambda(\xi)}{\partial\xi_\mu}d\xi+\langle\delta F\rangle.\tag{5·12}$$

Suppose now that $\langle F\rangle$ has n electron-open-polygons. Then $\langle F\rangle$ may be written in the following form, viz.

$$\langle F(x_1\cdots x_n, x_1'\cdots x_n')\rangle=\sum\int O^{(1)}(x_1u_1\cdots u_j\cdot x_1')\,O^{(2)}(x_2v_1\cdots v_k\cdot x_2')\cdots$$
$$\times\cdots O^{(n)}(x_nw_1\cdots w_l\cdot x_n')\cdot L(u_1\cdots u_jv_1\cdots v_kw_1\cdots w_l\eta_1\cdots\eta_mx_1\cdots x_n')\,du\cdot dvdwd\eta\,, \tag{5·13}$$

where $O^{(m)}$ represent the contribution from the m-th open-polygon and is defined by

$$O^{(1)}(x_1u_1\cdots u_jx_1')=S^F(x_1-u_1)\gamma^{\nu_1}S^F(u_1-u_2)\cdots S^F(u_{j-1}-u_j)\gamma^{\nu_j}S^F(u_j-x_1')\,, \tag{5·14}$$

and L represents the contribution from the remaining part of the diagram corresponding to $\langle F\rangle$. Finally the summation is carried over all the possible types of the diagrams. Here it is noted that if an S-vertex (at which $-\delta m\bar{\psi}\psi$ operates) lies on any one of open-polygons, γ^ν in (5·14) corresponding to this S-vertex must be put equal to 1.

The quantity $\delta\langle F\rangle/\delta\langle A_\mu(\xi)\rangle$ may be similarly expressed as

$$-\frac{i}{e_1}\frac{\delta\langle F\rangle}{\delta\langle A_\mu(\xi)\rangle}=\sum\sum_i\sum_j\int O^{(1)}(x_1\cdot u_1\cdots u_jx_1')\cdots O_\mu^{(i)}(x_ir_1\cdots r_{g-1}\xi\, r_g\cdots r_k\cdot x_i')$$
$$\cdots O^{(n)}(x_nw_1\cdots w_l\cdot x_n')$$
$$\times L(u_1\cdots u_j\cdots w_1\cdots w_k,\,\eta_1\cdots\eta_m\cdot x_1\cdots x_n')\,du\cdots dr\cdots dw\cdot d\eta$$
$$+\sum\int O^{(1)}\cdots O^{(n)}L_\mu(u\cdot v\cdots w\cdot\eta\cdot x_1\cdots x_n)\,du\,dv\,dw\,d\eta\,, \tag{5·15}$$

where the first term corresponds to the diagrams where the particular point ξ lies on the i-th open-polygon, and the second term corresponds to the diagrams where ξ lies on one of the closed loops. In (5·15), $O^{(h)}$ and L have similar expressions with those appeared in (5·13) and $O_\mu^{(i)}$ is given by

$$O_\mu^{(i)}(r_i\cdot r_1\cdots r_{g-1}\xi\, r_g\cdots r_k\cdot x_i')$$
$$=S^F(x_i-r_1)\gamma^{\nu_1}S^F(r_1-r_1)\cdots S^F(r_{g-1}-\xi)\gamma^\mu S^F(\xi-r_g)\cdots\gamma^{\nu_k}S^F(r_k-x_i')\,. \tag{5·16}$$

The factor L_μ in (5·15) may be written as

$$L_\mu=C_\mu L'\,, \tag{5·17}$$

where C_μ corresponds to the special closed loop C in which the vertex ξ is contained, and L' represents the contribution from the remaining part of the diagram corresponding to L_μ. Suppose that the closed loop C contains $m+1$ vertices ($m+1$ should be even on account of Furry's theorem) $\xi, Z_1\cdots Z_m$. Then C_μ may be written as

$$C_\mu(Z_1\cdots Z_h\cdot\xi\cdot Z_{h+1}\cdots Z_m)=\mathrm{tr.}[\gamma^{\rho_1}S^F(Z_1-Z_2)\gamma^{\rho_2}\cdots S^F(Z_h-\xi)\gamma_\mu S^F(\xi-Z_{h+1})$$
$$\cdots\gamma^{\rho_m}S^F(Z_m-Z_1)]\,.$$

Now bearing in mind the identity

$$\int \lambda(y) \frac{\partial}{\partial y_\mu} \{S^F(x-y)\gamma^\mu S^F(y-x')\}\, dy = S^F(x-x')\{\lambda(x)-\lambda(x')\}, \qquad (5\cdot18)$$

we can easily verify the equation

$$\int d\xi \lambda(\xi) \sum_{h=0}^{m-1} \frac{\partial}{\partial \xi_\mu} C_\mu(Z_1 \cdots Z_h \cdot \xi \cdot Z_{h+1} \cdots Z_m) = 0 \qquad (5\cdot19)$$

where $Z_0 = Z_m$ is supposed. Substituting from (5·15), (5·17) and (5·19) into (5·12), we have

$$\delta\langle F\rangle = \langle \delta F\rangle + (-ie_1)\sum_{(i,g)}\sum \int O^{(1)} \cdots \frac{\partial O_\mu^{(i)}(x_i r_1 \cdots r_{g-1} \cdot \xi \cdot r_g \cdots r_k \cdot x_i')}{\partial \xi^\mu} \cdots O^{(n)} \cdot L\lambda(\xi)\, du \cdots dw \cdot d\eta \cdot d\xi. \qquad (5\cdot20)$$

Since the relation

$$\int d\xi \lambda(\xi) \frac{\partial O_\mu^{(i)}(x_i r_1 \cdots r_{g-1} \xi r_g \cdots r_k x_i')}{\partial \xi_\mu} = -\{\lambda(r_{g-1}) - \lambda(r_g)\} O^{(i)}(x_i r_1 \cdots r_k x_i')$$

holds by means of (5·18), we get

$$\sum_{g=1}^{k+1} \int d\xi \lambda(\xi) \frac{\partial}{\partial \xi_\mu} O_\mu^{(i)}(x_i r_1 \cdots r_{g-1} \xi r_g \cdots r_k x_i') = -\{\lambda(x_i) - \lambda(x_i')\} O^{(i)},$$

where $r_0 = x_i$ and $r_{k+1} = x_i'$ are assumed. Therefore $\langle \delta F\rangle$ may be written as

$$\delta\langle F\rangle = ie_1 \sum_{i=1}^{\infty} \{\lambda(x_i) - \lambda(x_i')\}\langle F\rangle + \langle \delta F\rangle \qquad (5\cdot21)$$

by virtue of the expression (5·13). Comparing (5·21) with (5·12), we get the relation

$$\int \frac{\delta\langle F\rangle}{\delta\langle A_\mu(\xi)\rangle} \frac{\partial \lambda(\xi)}{\partial \xi_\mu} d\xi = ie_1 \sum_{i=1}^{n} \{\lambda(x_i) - \lambda(x_i')\}\langle F\rangle. \qquad (5\cdot22)$$

All the equations (5·2)–(5·8) can be easily derived from (5·21). For instance, if we put F equal to $iT(\psi\bar{\psi})$, then $\langle F\rangle$ becomes G itself. Since G has a single open-polygon, and $\delta \cdot T(\psi\bar{\psi})$ is equal to zero, we have the equation such as

$$\delta\langle G\rangle = ie_1\{\lambda(x) - \lambda(x')\} G .$$

This is just the equation (5·2) represented in case of the infinitesimal gauge transformation. Further, if we put F equal to A_μ, then $\langle F\rangle$ turns into $\langle A_\mu\rangle$. In this case (5·21) may be written as

$$\delta\langle A_\mu(x)\rangle = \left\langle \frac{\partial \lambda}{\partial x_\mu} \right\rangle = \frac{\partial \lambda}{\partial x_\mu},$$

because $\langle A_\mu\rangle$ has no open-polygons. Furthermore, if we take $\sum^*$ for $\langle F\rangle$, (5·22) runs to

$$\int \frac{\delta \sum^*}{\delta\langle A_\mu(\xi)\rangle} \frac{\partial \lambda(\xi)}{\partial \xi_\mu} d\xi = ie_1\{\lambda(x) - \lambda(x')\}\sum^*$$

which is just the equation (5·9) by means of $(4\cdot8)_c$.

We have so far only concerned with the unprimed quantities. However if we take account of the transformation

$$\lambda \to \lambda' = \frac{1}{\sqrt{a}}\lambda ,$$

all the results obtained in this section are also true in case of the primed quantities.

§ 6. Concluding remarks

Since our argument is essentially based on the assumption of expandability in powers of the coupling constant, it runs counter to Schwinger's intention. However all the equations such as (4·7)–(4·12), can be also derived from the Tomonaga-Schwinger theory without using the assumption of expandability (*c.f.* appendix). Thus these equations can be considered to have no relations to this assumption as already shown by Schwinger. From this standpoint, however, the physical meaning of several quantities is not comprehensible till these equations are solved in some way. On the other hand, following our line of reasoning, these meanings become obvious in the course of derivation of the fundamental equations. This fact is a favourable point gained by sacrificing the independence of the theory upon the assumption of expandability. Further in the present stage of physics, it seems to be impossible to give a proof of removability of divergences without relying on the expandability in terms of e.

Accordingly in order to attain Schwinger's object, it is most desirable to prove the existence of a well-behaved solution of the system of integro-differential equations (4·14)–(4·23), without use of the expandability.

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Appendix 1

In Dyson's paper somewhat lengthy remarks are given about the so-called normal-dependent term of the Hamiltonian (4·5). We shall give a short remark about the treatment of this term.

The Hamiltonian (4·5) may be written as

$$H = H' - \delta\dot{m}\bar{\psi}\psi - A_\mu(J_\mu + j_\mu) \qquad (4\cdot5)$$

with the substitution

$$H' = -\frac{f}{4}F_{kl}F_{kl} - \frac{f'}{2}F_{k4}F_{k4} . \qquad (a\cdot1)$$

We shall often encounter problems of evaluating the expression $\langle F \rangle$, where F is any operator in the interaction representation. $\langle F \rangle$ may be expressed as

$$\langle F\rangle = -\int \langle F j_\mu(x) j_\nu(x')\rangle' K_{\mu\nu}(xx')\,dx\,dx', \tag{a·2}$$

where

$$K_{\mu\nu}(xx') = \sum_0^\infty \frac{(-i)^n}{n!}\int (0|T(A_\mu(x)A_\nu(x')H'(y_1)\cdots H'(y_n))|0)\,dy_1\cdots dy_n. \tag{a·3}$$

Of course the factor $\langle F j_\mu j_\nu\rangle'$ involves many $K_{\mu\nu}$'s, namely it is written as

$$\langle F j_\mu j_\nu\rangle' = \Psi_{\mu\nu}[x, x', F, K].$$

If $f=0$ as in case of §§ 1–3, the Hamiltonian is invariant in this case, and $K_{\mu\nu}$ turns to

$$(A_\mu(x)A_\nu(x')) = \delta_{\mu\nu}D^F(x-x'),$$

and $\langle F\rangle$ becomes

$$-\int \Psi_{\mu\mu}[x, x', F, D^F]D^F(x-x')\,dx\,dx'. \tag{a·4}$$

It is easily seen that (a·2) can be derived from (a·4) by placing arbitrary number of H''s on every photon line appearing in the diagrams corresponding to (a·4).

Now in order to prove the invariance of $\langle F\rangle$ (i. e. the normal-independence) it is sufficient to show $K_{\mu\nu}$ being normal-independent.

Following the treatment explained in §§ 1–3, we can express $K_{\mu\nu}$ in the following way by analysing the right-hand side of (a·3),

$$\begin{aligned} K_{\mu\nu}(xx') = \int D^F(x-y)\Big[&\delta(y-x')\delta_{\mu\nu} - if\delta_{\mu k}\frac{\partial^2}{\partial y_i^2}K_{k\nu}(yx') \\ &+ if\delta_{\mu k}\frac{\partial^2}{\partial y_k\partial y_l}K_{l\nu}(yx') - if'\delta_{\mu k}\frac{\partial}{\partial y_4}K'_{k\nu}(yx') - if'\delta_{\mu 4}\frac{\partial^2}{\partial y_i^2}K_{4\nu}(yx') \\ &+ if'\delta_{\mu 4}\frac{\partial}{\partial y_k}K'_{k\nu}(yx') + if'\delta_{\mu k}\frac{\partial^2}{\partial y_4\partial y_k}K_{4\nu}(yx')\Big]dy, \end{aligned} \tag{a·5}$$

where $K'_{k\nu}$ is defined by

$$K'_{k\nu}(xx') = \sum_0^\infty \frac{(-i)^n}{n!}\int (0|T\left\{\frac{\partial A_k(x)}{\partial x_4}A_\nu(x')H'(y_1)\cdots H'(y_n)\right\}|0)\,dy_1\cdots dy_n. \tag{a·6}$$

$K'_{k\nu}$ can be also expressed in the following way by using the same method as in (a·5) and taking account of the definition of $K_{\mu\nu}$ itself,

$$\frac{1}{1-f}K'_{k\nu} = \frac{\partial K_{k\nu}}{\partial x_4} + f'\frac{\partial K_{4\nu}}{\partial x_k}. \tag{a·7}$$

Here the relation

$$\left(\frac{\partial A_\mu(x)}{\partial x_4}\frac{\partial A_\nu(x')}{\partial x_4'}\right) = \frac{\partial^2}{\partial x_4\partial x_4'}(A_\mu(x)A_\nu(x')) + i\delta_{\mu\nu}\delta(x-x')$$

is in use. Substituting back (a·7) into (a·6), we get

$$K_{\mu\nu}(xx')=\delta_{\mu\nu}D^F(x-x')+if\int D^F(x-y)\left(\frac{\partial^2}{\partial y_\mu\partial y_\rho}-\delta_{\mu\rho}\Box\right)K_{\rho\nu}(yx')\,dy\,. \tag{a·8}$$

Taking the four-dimensional divergence of (a·5) with regard to x_μ, we have

$$\frac{\partial K_{\nu\mu}}{\partial x_\mu}=\frac{\partial D^F(x-x')}{\partial x_\nu}\,. \tag{a·9}$$

Substitute from (a·9) again into (a·8), then we have finally

$$K_{\mu\nu}(xx')=\frac{1}{1-f}\delta_{\mu\nu}D^F(x-x')+if'\int D^F(x-y)\frac{\partial^2}{\partial y_\mu\partial y_\nu}D^F(y-x')\,dy\,. \tag{a·10}$$

Thus it has become clear that $K_{\mu\nu}$ is independent on the time-direction. It is noted that the adoption of the Hamiltonian (4·5) instead of

$$-\delta m\bar{\psi}\psi-A_\mu(J_\mu+j_\mu)$$

means not only a simple renormalization such as

$$\begin{aligned}\delta_{\mu\nu}D^F(x-x')&=(A_\mu^*(x),\,A_\nu^*(x'))\to\frac{1}{1-f}\delta_{\mu\nu}D^F(x-x')\\&=(\theta A_\mu^*(x),\,\theta A_\nu^*(x'))=(A_\mu(x)A_\nu(x')),\end{aligned} \tag{a·11}$$

but also a new type of renormalization corresponding to the second term in (a·10).

On the other hand if we adopt a Lagrangian density L^* expressed in terms of renormalized quantities, such as

$$\begin{aligned}L^*=&-\frac{1}{4}F_{\mu\nu}F_{\mu\nu}-\frac{1}{2}\left(\frac{\partial A_\mu}{\partial x_\mu}\right)^2+L_D+L_{\text{int}}+\frac{f}{4}F_{\mu\nu}F_{\mu\nu}\\&+\delta m\bar{\psi}\psi+\frac{f}{4}F_{\mu\nu}F_{\mu\nu}+\frac{f}{2}\left(\frac{\partial A_\mu}{\partial x_\mu}\right)^2=L+\frac{f}{2}\left(\frac{\partial A_\mu}{\partial x_\mu}\right)^2,\end{aligned} \tag{a·12}$$

L being given by (4·4), then the interaction Hamiltonian corresponding to L^* becomes

$$\begin{aligned}\mathfrak{H}&=H-\frac{f'}{2}\left(\frac{\partial A_\mu}{\partial x_\mu}\right)^2\\&=\mathfrak{H}'-\delta m\bar{\psi}\psi-A_\mu(J_\mu+j_\mu)\end{aligned} \tag{a·13}$$

with the substitution

$$\mathfrak{H}'=H'-\frac{f'}{2}\left(\frac{\partial A_\mu}{\partial x_\mu}\right)^2. \tag{a·14}$$

In this case $K_{\mu\nu}$ turns into

$$K_{\mu\nu}=\frac{1}{1-f}\delta_{\mu\nu}D^F(x-x'), \tag{a·15}$$

and the equation statisfied by $\mathfrak{G}_{\mu\nu}$ is given by

$$\{\Box\delta_{\mu\rho}-(P_{\mu\rho}+f\Box\delta_{\mu\rho})\}\mathfrak{G}_{\rho\nu}=-\delta_{\mu\nu} \tag{a·16}$$

instead of (4·10). The adoption of the Lagrangian (a·12) corresponds to the simple renormalization (a·11) as easily seen from (a·15). The expression (a·16) is insufficient to remove the divergences arising in $P_{\mu\rho}$ by virtue of the very character given in page 97. Thus the difference between L and L^* is essential for the removability of divergences in the theory of Green-functions. In case of (a·16), the remaining divergence of $P_{\mu\nu}$ has the expression

$$-Ak_\mu k_\nu$$

in the momentum representation. Fortunately this divergence disappears in the theory of S–matrix on account of the conservation of charge and the Lorentz condition. Therefore L^* is effectively equivalent to L in the theory of S–matrix.

Appendix 2

We shall derive the equation (2·6) from the Tomonaga-Schwinger theory without use of the assumption of expandability in powers of e.

The transformation function $S(t_1 t_2)$ between t_1 and t_2 are defined by

$$i\frac{dS(t_1 t_2)}{dt_1} = \int H(\vec{x}_1 t_1) d\vec{x}_1 \, S(t_1 t_2), \tag{b·1}$$

with the initial condition $S(t_2 t_2) = 1$.

This equation may be transformed into an integral equation

$$S(t_1 t_2) = 1 - i\int_{t_2}^{t_1} H(x') S(t' t_2) dx'. \tag{b·2}$$

From this we have

$$\frac{\delta S(t_1)}{\delta J_\mu(\xi)} = \left\{ \begin{array}{ll} +iA_\mu(\xi) S(\xi_0) - i\int_{\xi_0}^{t_1} H(x') \dfrac{\delta S(t')}{\delta J_\mu(\xi)} dx', & t_1 > \xi_0, \\ 0, & \xi_0 < t_1 \end{array} \right\} \tag{b·3}$$

with the notation $S(x_1) \equiv S(t_1, t_2 = -\infty)$.

Multiply $iA_\mu(\xi) S(t_2)$ to (b·2) from the right-side, then we get

$$iS(t_1 \xi_0) A_\mu(\xi) S(\xi_0) = iA_\mu(\xi) S(\xi_0) - i\int_{\xi_0}^{t_1} H(x') iS(t' \xi_0) A_\mu(\xi) S(\xi_0) dx', \tag{b·4}$$

where t_2 is supposed to be equal to ξ_0.

Comparing (b·4) with (b·3), we obtain

$$\frac{\delta S(t_1)}{\delta J_\mu(\xi)} = \left\{ \begin{array}{ll} iS(t_1 \xi_0) A_\mu(\xi) S(\xi_0) = iS(t_1) \boldsymbol{A}_\mu(\xi), & t_1 > \xi_0, \\ 0, & \xi_0 > \xi_1 \end{array} \right\}. \tag{b·5}$$

Now any Heisenberg operator $\boldsymbol{F}(x)$ can be represented in the interaction representation, as

$$\boldsymbol{F}(x) = S^{-1}(x_0) F(x) S(x_0).$$

From this we get

$$\frac{\delta \boldsymbol{F}(x)}{\delta J_\mu(\xi)} = \begin{cases} i[\boldsymbol{F}(x),\ \boldsymbol{A}_\mu(\xi)], & x_0 > \xi_0, \\ 0, & \xi_0 > x_0 \end{cases} \qquad (b\cdot 6)$$

by means of (b·5), provided that F is independent on J.

The Green-function G of one-electron problem can be expressed in the Heisenberg representation as

$$G = i(\Psi^*_{\text{vac}} \cdot ST(\psi(x')\bar{\psi}(x'))\Psi_{\text{vac}})/S_{\text{vac}} .$$

Since ψ satisfies the equation

$$[\gamma^\mu\{-i\partial_\mu - e\boldsymbol{A}_\mu(x)\} + m]\psi(x) = 0 ,$$

G satisfies the equation

$$[\gamma^\mu(-i\partial_\mu) + m]G = i(\Psi^*_{\text{vac}} ST\{e\boldsymbol{A}_\mu(x)\gamma^\mu\psi(x),\ \bar{\psi}(x')\}\Psi_{\text{vac}})/S_{\text{vac}} + \delta(x-x'). \qquad (b\cdot 7)$$

Now by means of (b·5) and (b·6), we have

$$\frac{\delta G(xx')}{\delta J_\mu(\xi)} = -(\Psi^*_{\text{vac}} S \cdot T(\psi(x)\bar{\psi}(x')\boldsymbol{A}_\mu(\xi))\Psi_{\text{vac}})/S_{\text{vac}} - iG\langle A_\mu(\xi)\rangle, \qquad (b\cdot 8)$$

where $\langle A_\mu(\xi)\rangle$ is defined by

$$\langle A_\mu(\xi)\rangle = (\Psi^*_{\text{vac}} S\boldsymbol{A}_\mu(\xi)\Psi_{\text{vac}})/S_{\text{vac}} ,$$

which agrees with the definition in (1·9).

Substitute from (6·8) into (6·7), we get

$$\left[\gamma^\mu(-i\partial_\mu - e\langle A_\mu(x)\rangle) + m + ie\gamma^\mu \frac{\delta}{\delta J_\mu(x)}\right] G(xx') = \delta(x-x'). \qquad (b\cdot 9)$$

This is just the equation (2·6).

All the other equations in §§ 1–4 can be similarly derived.

Here it must be noted that in deriving (b·7) the adiabatic assumption is neccessary. This situation will be made obvious if we define G in the following way:

$$G(xx') = i(\Psi^*_{\text{vac}} S(T_0, -T_0)\, T(\psi(x)\bar{\psi}(x'))\Psi_{\text{vac}})$$

instead of

$$G = i(\Psi^*_{\text{vac}} S(\infty, -\infty)\, T(\psi(x)\bar{\psi}(x'))\Psi_{\text{vac}}).$$

References

1) J. Schwinger, Proc. N.A.S. **37** (1951), 452.
2) J. Schwinger, Phys. Rev. **82** (1951), 914.
3) F. J. Dyson, Phys. Rev. **75** (1949), 1736.
4) G. C. Wick, Phys. Rev. **80** (1950), 268.
5) M. Gell-Mann and F. Low, Phys. Rev. **84** (1951), 350.
6) F. J. Dyson, Phys. Rev. **83** (1951), 608.
7) S. N. Gupta, Proc. Phys. Soc. (London) A **64** (1951), 426.
8) J. C. Ward, Phys. Rev. **78** (1950), 182 (L).

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On The Inelastic Collision between Molecules, I

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The energy transfer between the vibration and the translation in the molecular collision is investigated for the linear configuration of two diatomic molecules. The method of calculation is completely parallel to that of Jackson and Mott. The results are applied to the interpretation of the experimental facts for the anomalous supersonic dispersion and the qualitative successes are obtained.

§ 1. Introduction

As is well known, quantum mechanics has been established firmly in the region of atoms or molecules. However, the theory of molecular collisions (especially of inelastic ones) presents so large mathematical difficulty that it has been studied only rarely. But the molecular collisions play the important role in the various phenomena, e.g. the discharge in gas, the phenomena in the ionosphere, the chemical reaction in general, the anomalous supersonic dispersion, and so on. Thus it is desirable to investigate more closely the various elementary processes in the molecular collisions.

In this paper we treat the energy transfer between the vibrational and the translational degrees of freedom in the collision of simple molecules with each other, and apply the results to explain the experimental facts relating to the anomalous supersonic dispersion. Problems of this kind were examined twenty years ago by Zener[1], who discussed the coupling of the translation with the vibration or the rotation. Subsequently a more mathematically refined treatment was proposed by Jackson and Mott[2] in connection with the calculation of the accommodation coefficient. These authors, however, did not consider the possibility that the vibrational energy of the one molecule may be transfered not only to the translation but also to the vibration of the other molecule by the collision. Such a process is studied in this paper. The method of the calculation is completely parallel to that used by Jackson and Mott.

Now the influence of the collision partner for the deactivation of the molecule considered may be classified as follows:

1. the effect of the molecule as a whole (dependence on mass and size).
2. the effect of the rotation (possibility of taking off a part of the excess energy by the rotational degrees of freedom).
3. the effect of the vibration (effect similar to the above, by the vibrational degrees of freedom).
4. the electronic effect (dependence on the form of the intermolecular force. If the

collision partners can (at least in principle) react chemically with each other, then the intermolecular force potential will have very different feature from the other cases). The possibility of the excitation of electronic states will play no important role in the thermal collision at ordinary temperature.

In this paper, we touch the effects 1 and 2 only briefly, and do not enter into the effect 4. For the estimation of the vibrational effect, we furthermore restrict ourselves to the linear configuration of two diatomic molecules without rotation, as shown in Fig. 1(a). More generally, if the transition probabilities for the configurations of Fig. 1 (a), (b) and (c) are p_a, p_b and p_c respectively, we may assume that the transition probability for the case of the collision in the general configuration of Fig. 1 (d) is given by a suitable interpolation, e.g.

$$p_d = p_a\left(\cos^2\theta_1 + \frac{p_c}{p_a}\sin^2\theta_1\right)\left(\cos^2\theta_2 + \frac{p_b}{p_a}\sin^2\theta_2\right),$$

without any serious error.

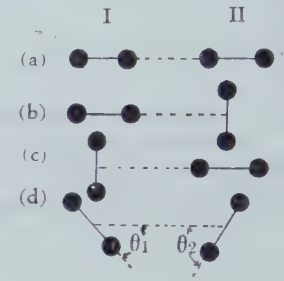

Fig. 1.

Now for the vibration-vibration coupling the transition probability will be comparatively large for the configuration of Fig. 1(a), and for other configurations it will be very much smaller. Thus we may put roughly

$$p_d \cong p_a \cos^2\theta_1 \cos^2\theta_2,$$

and by averaging over the angles θ_1 and θ_2 we have

$$\bar{p}_d \cong p_a/9.$$

Therefore, if we write the average transition probability as $p_a p_0$, then p_0 is order of magnitude of 10^{-1} and when we are interested in the relative probability only, it is sufficient to know the factor p_a, i.e., the transition probability for the special configuration (a).

The results of our calculations show that the final result is very sensitive to the choice of the parameter contained in the perturbation potential. (See Fig. 3 and 4.) Thus we have to investigate the potential curve for each special case. This problem, as well as several related problems will be considered in subsequent papers.

§ 2. Effect of a molecules as a whole*

First of all, the difference in geometrical extension will necessarily cause the difference in the effective cross section for the transition investigated, although these two cross sections are not always proportional to each other.

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* Atomic units are used throughout this paper. Thus, for example, electron mass$=1$, $\hbar=1$, and the energy quantum $h\nu(=\hbar\omega)$ has the same numerical value as the angular frequency ω.

In the second place, the difference of the mass of the collision partner causes the change of the reduced mass (μ) for the total system. If the energy transfered from the vibrational to the translational degrees of freedom is equal to ΔE, then

$$E=\frac{k^2}{2\mu}\,;\quad \Delta E=\frac{(k+\Delta k)^2-k^2}{2\mu}=\sqrt{2E}\left(\frac{\Delta k}{\sqrt{\mu}}\right)+\frac{1}{2}\left(\frac{\Delta k}{\sqrt{\mu}}\right)^2.$$

Now the average relative translational energy for each collision, which is derived from the Maxwellian velocity distribution, is $\bar{E}=2kT$, independent of the reduced mass. Thus, for the fixed value of ΔE, we have $\Delta k\propto\sqrt{\mu}$. Since the large change of the wave number k means the small overlapping between the initial and the final translational wave functions, the smallness of the reduced mass is in favour of the large transition probability (provided the other conditions unchanged). From the experimental evidence for the anomalous supersonic dispersion, we know that the He-atom, though it has neither vibrational nor rotational degrees of freedom, is more effective for the deactivation of O_2 compared with O_2 itself. This will be explained by the fact that the ratio of reduced masses for the two systems O_2-O_2 and O_2-He is 9 : 2. As another example, the experimental fact[3] that the ratio of the effectiveness (transition probability per collision) of H_2 and D_2 for the deactivation of the vibration of CO_2 is 3 : 1 can be explained only by taking the difference of the reduced mass into account.

§ 3. Effect of the rotation

Generally, the rotational level spacings are much smaller than the vibrational ones. Therefore, in order that the rotational degrees of freedom may take off the great part of excess energy after vibrational deactivation, a large change of the rotational quantum number must necessarily occur which is improbable. However, if the rotational level spacings are comparatively large (as in the case of H_2 and HCl etc.), the rotation may have appreciable effects on the deactivation of vibration. The experimental fact that HCl is considerably effective for the vibrational deactivation of CO_2, Cl_2 etc., may be explained by the large rotational level spacings of HCl, though the explanation that this effectiveness is due to the special form of the intermolecular force is also possible. The large rotational level spacing, on the other hand, gives rise to the rotational supersonic dispersion.[4] The treatment of this problem will be postponed to a later article.

§ 4. Effect of the vibration

It is well known that Born approximation is not valid for the slow atomic collisions. However, the transition probability between the vibration of one molecule and the vibration of another molecule is known experimentally to be very small. Therefore, the method of distorted wave may be applied.

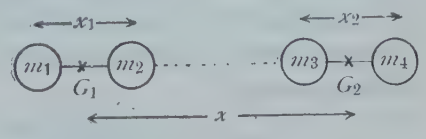

Fig. 2 $\sum m_i$: atomic masses
G_i : gravity-center of each molecule

As stated in the introduction, we consider

the special configuration which is illustrated by Fig. 2. The independent variables are x_1, x_2 and x as shown in Fig. 2. The Schrödinger's wave equation for the whole system is as follows

$$[-H^{(1)}-H^{(2)}+(1/2\mu)\partial^2/\partial x^2+(W-V)]\Psi(x\,;z_1,z_2)=0,$$

where

$$H^{(i)}=-(1/2\mu_i)\partial^2/\partial z_i^2+2\pi^2\mu_i\nu_i^2 z_i^2,$$

$$z_i=x_i-\bar{x}_i,$$

and

$$\mu_1=m_1m_2/(m_1+m_2),\quad \mu_2=m_3m_4/(m_3+m_4),$$

$$\mu=(m_1+m_2)(m_3+m_4)/(m_1+m_2+m_3+m_4).$$

Here, we adopt the exponential form for the potential energy :

$$V=C_0\exp\{-a(x-\lambda_1x_1-\lambda_2x_2)\}$$
$$=C\exp(-ax)\exp(a\lambda_1z_1)\exp(a\lambda_2z_2),$$

where $\lambda_1=m_1/(m_1+m_2),\qquad \lambda_2=m_4/(m_3+m_4).$

$H^{(i)}$ is the well-known Hamiltonian operator for the harmonic oscillator and we represent its normalized eigenfunctions by $\psi_n^{(i)}(z_i)$, which satisfy

$$H^{(i)}\psi_n^{(i)}(z_i)=\left(n+\frac{1}{2}\right)\omega_i\psi_n^{(i)}(z_i).$$

Now we seek for the solution of the form :

$$\Psi=\sum_{n,m}f_{n,m}(x)\psi_n^{(1)}(z_1)\psi_m^{(2)}(z_2).$$

If the molecule 1 is in the first excited state before collision, then we must impose the asymptotic conditions

$$f_{1,0}\overset{x\to\infty}{=}\exp(-ik_{1,0}x)+A_{1,0}\exp(ik_{1,0}x),$$

$$f_{n,m}\overset{x\to\infty}{=}A_{n,m}\exp(ik_{n,m}x),\quad (n,m)\neq(1,0).$$

Then the transition probability per collision is given by

$$p_{1,0}^{n,m}=(k_{n,m}/k_{1,0})|A_{n,m}|^2.$$

The method used for the determination of $A_{n,m}$ is similar to that of Jackson and Mott[2] who considered the collision problem between a harmonic oscillator and an inert gas atom. Completely parallel calculations give the following result which corresponds to the Eq. (19) of these authors,

$$p_{1,0}^{n,m}=\frac{4(Y_{1,n}^{(1)})^2(Y_{0,m}^{(2)})^2}{k_{1,0}k_{n,m}}\left[2\mu C\cdot\int_{-\infty}^{\infty}F_{1,0}F_{n,m}\exp(-ax)\,dx\right]^2,$$

where

$$Y_{s,t}^{(i)}=\int_{-\infty}^{\infty}\psi_s^{(i)}(z_i)\psi_t^{(i)}(z_i)\exp(a\lambda_i z_i)dz_i,$$

and F is the solution of

$$[d^2/dx^2+k_{n,m}^2-2\mu C\cdot\exp(-ax)]F_{n,m}(x)=0,$$

which approaches zero for $x\to-\infty$ and behaves asymptotically as $\cos(k_{n,m}x+\eta_j)$ for $x\to+\infty$. The explicit form of this F-function and the integral containing this function were obtained by Jackson and Mott, and the use of their results gives the final expression for the transition probability

$$P_{1,0}^{n,m}=\frac{\pi^2}{4}(Y_{1,n}^{(1)})^2(Y_{0,m}^{(2)})^2\left[\frac{q_{n,m}^2-q_{1,0}^2}{\cosh\pi q_{n,m}-\cosh\pi q_{1,0}}\right]^2\sinh\pi q_{n,m}\sinh\pi q_{1,0}, \qquad (1)$$

where $q_{n,m}=2k_{n,m}/a$. The vibrational matrix elements $Y_{s,t}$ are easily calculated for small s, t and are as follows:

$$Y_{0,0}^{(i)}=\exp(a^2\lambda_i^2/4a_i)\cong 1,$$

$$a_i=\mu_i\omega_i, \qquad (2)$$

$$Y_{1,0}^{(i)}=a\lambda_i/(2a_i)^{1/2}\times\exp(a^2\lambda_i^2/4a_i).$$

Numerical examples for the case of $\lambda=1/2$ (homonuclear diatomic molecule) and $a=1$, 3, 5 are shown in Fig. 3.

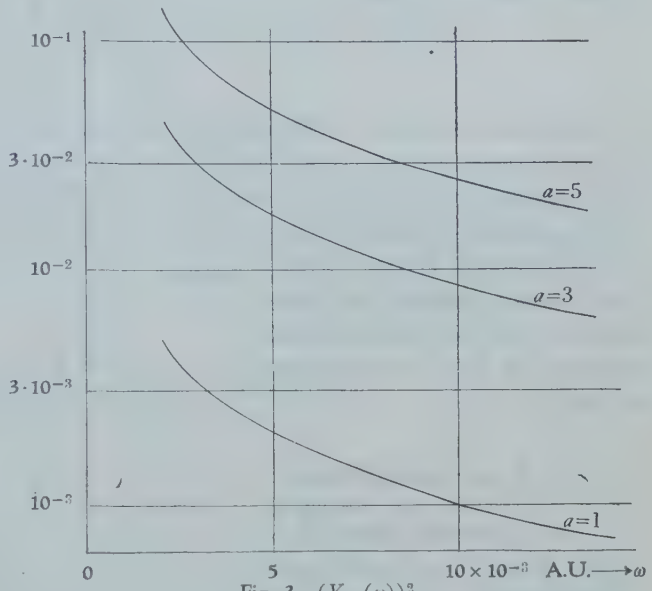

Fig. 3 $(Y_{1,0}(\omega))^2$.
$(\lambda=1/2,\ \mu=1.25\times10^4)$

Next, we consider the remaining important factor

$$I_{n,m}=\left(\frac{q_{n,m}^2-q_{1,0}^2}{\cosh\pi q_{n,m}-\cosh\pi q_{1,0}}\right)^2\sinh\pi q_{n,m}\sinh\pi q_{1,0}. \qquad (3)$$

Usually q is much larger than unity and in this case we may put

$$I_{n,m}=\left(\frac{q_{n,m}^2-q_{1,0}^2}{\exp(\pi q_{n,m})-\exp(\pi q_{1,0})}\right)^2\exp(\pi q_{n,m})\exp(\pi q_{1,0}). \qquad (3a)$$

Moreover, if $\exp(\pi q_{n,m})\gg\exp(\pi q_{1,0})$, we have

$$I_{n,m}=(q_{n,m}^2-q_{1,0}^2)^2\exp(\pi q_{1,0})/\exp(\pi q_{n,m}). \qquad (3b)$$

In this last approximation, we obtain, using the definition of q, that

$$I_{n,m} \propto \Delta E \cdot \exp\{-\text{const} \cdot \Delta E/(k_{n,m}+k_{1,0})\}. \tag{4}$$

Thus, if the initial translational energy becomes large, also the transition probability becomes large.

Now the energy conservation relation is expressed by

$$k_{n,m}^2 + 2\mu(n\omega_1 + m\omega_2) = k_{1,0}^2 + 2\mu\omega_1.$$

If we fix the initial wave number $k_{1,0}$, the matrix element $I_{n,m}$ is a function of energy change $\Omega\ (\equiv(k_{n,m}^2 - k_{1,0}^2)/2\mu)$ and is independent of n and m. Numerical examples for $I(\Omega)$ for the case of $k_{1,0}=10$, which corresponds to O_2, N_2 etc, at room temperature, are illustrated by Fig. 4.

Now we may expect that the exact resonance case $(\Omega=0)$ is the maximum point of the function $I(\Omega)$. But it is only approximately true. Since the expansion of this function near $\Omega=0$ gives

$$I = \frac{4}{\pi^2} q_{1,0}^2 + \frac{4}{\pi^2} q_{1,0}(q_{n,m} - q_{1,0}) + O((q_{n,m}-q_{1,0})^2), \tag{5}$$

the maximum point of this function is shifted to a positive value of $\Omega\ (q_{n,m} > q_{1,0})$.

A characteristic feature of the function I is the very rapid decrease for the increase of its argument Ω, which is a marked contrast to the comparatively slow variation of $V_{s,t}$. As a result, the two quanta process $(1,0)\rightarrow(0,1)$ may become much more probable than the one quantum process $(1,0)\rightarrow(0,0)$ which explains the various effects for the anomalous supersonic dispersion in gases. (See the next section.)

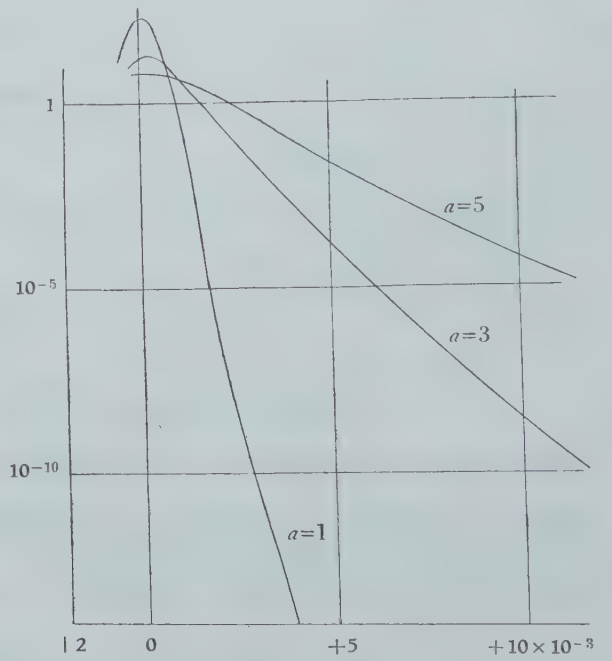

Fig. 4 $I(\Omega)$ $k_{\text{initial}}=10$, $2M=5\times10^4$

§ 5. Some applications

The numerical values shown in Fig. 3 and 4 correspond to the special choice of the parameters. For the simple molecules consisting of atoms with nearly equal masses such as O_2, N_2, CO, CO_2, NO, N_2O etc., these figures may be used to make qualitative discussions, because the difference of the vibrational frequencies will be the most dominant factor there.

O_2.....($\omega=7.2\times10^{-3}$ atomic units) The transfer of the vibrational energy of O_2 to the vibrational

energy of another O_2 is an example of the exact resonance, and therefore has a comparatively large probability. But such transfer can not be detected experimentally. On the other hand the probability of energy transfer to the translation is 3×10^{-8} (using the values from Fig. 3 and 4, provided $a=3$). Since it is not the vibration-vibration coupling, the extra factor p_0 discussed in the introduction may be put as 1/3 instead of 1/10. Thus the average number Z of collisions occuring before the deactivation of vibrational excitation is about 10^8 which is compared with the experimental value[5] $Z>5\times10^6$.

From the experimental evidences[5] we know that the molecules such as N_2, CO etc. are more effective than O_2 itself, though they have large vibrational frequencies. This may be ascribed to the difference of potential curves for the individual cases. In fact, the transition probability varies over a comparatively wide range for a small variation of the parameter a. (See Fig. 3 and 4.)

N_2O.....This molecule has the following three modes of vibration:

1. deformation vibration: $\omega_1=2.7\times10^{-3}$,
2. valence vibration (symmetrical): $\omega_2=5.9\times10^{-3}$,
3. valence vibration (antisymmetrical): $\omega_3=10.2\times10^{-3}$.

When two N_2O molecules collide with each other, a possible process is that the valence vibration of the one N_2O is deactivated while the deformation vibration of the other N_2O is activated. In this way, the three modes of vibration are not independent of each other. The transition probabilities (however, only relative) between various levels of N_2O are shown in Fig. 5. Here we have used the approximate relations:[6][7]

$$\frac{\text{probability for the transition : } n\text{-th level}\rightarrow(n-1)\text{th level}}{\text{probability for the transition : 2nd level}\rightarrow\text{1st level}}=2n-1,$$

$$\text{Probability for the transition : } n\text{-th level}\rightarrow\text{1st level}$$

$$=(\text{probability for the transition : 2nd level}\rightarrow\text{1st level})^{n-1}.$$

From this diagram we can see that the deactivation probability of the symmetric valence vibration increases by factor of 500 by coupling with the 2nd excited state of the deformation vibration, and very much approaches to the deactivation probability of the deformation vibration itself. Thus we may hope that the experimental evidence of Eucken-Nümann[8] can be explained by this coupling effect. (They found that the relaxation times for the deformation and the valence vibration are not so different as by factor 10 with each other.)

From Fig. 5, we can also see that the deactivation probability of the antisymmetric valence vibration is much different from that of the other two modes of vibration. However, the antisymmetric valence vibration contributes only a little to the dispersion phenomena in the room temperature and the separation of the two maxima of dispersion can not be tested. Thus, it is desirable to investigate experimentally the supersonic dispersion at higher temperature (for example 300°C or more).

CO_2.....The behavior of CO_2 is completely analogous to that of N_2O and, therefore, only the transition diagram is shown (Fig. 6).

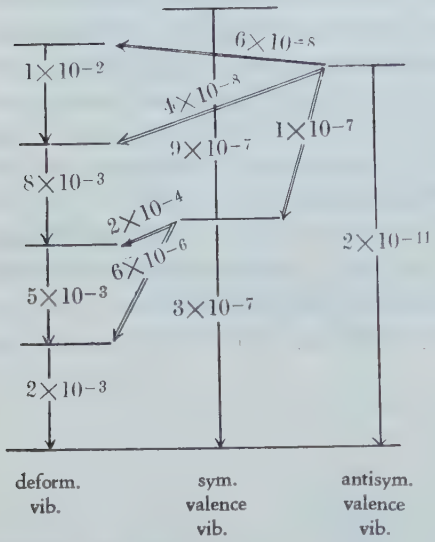

Fig. 5 Case of N_2O.

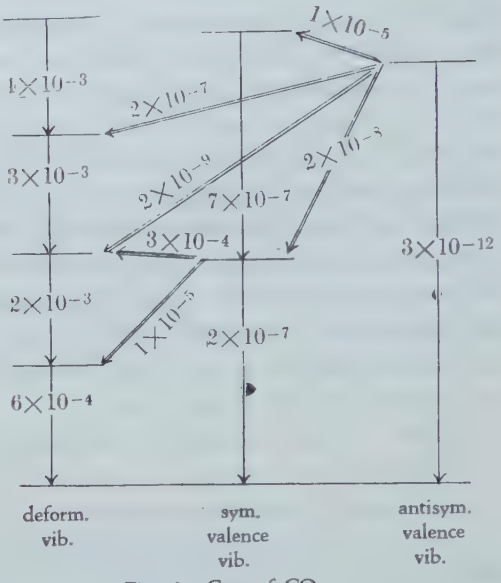

Fig. 6. Case of CO_2.

Single line ⟶ transition probability (relative scale) from any vibrational level to the next lower one belonging to the same type (and in the same molecule), by a collision with another molecule.

double line ⟹ transition probability for the process that a type of vibration of the one molecule is deactivated to the ground state and, at the same time, another type of vibration of the other molecule (collision partner) is activated from the ground state.

§ 6. Conclusions

Since the calculations performed in this paper are accompanied with many simplifications, we cannot obtain the quantitative conclusions from them. However, it is not so unreasonable to believe that the general principle explaining the experimental facts has been obtained. In other words, the ordinary method of distorted wave seems to give a satisfactory way of calculation.

The main articles which will be investigated in the following papers are:

1) More quantitative calculations for some special cases (The intermolecular force potential has to be calculated for each case quantummechanically. The general geometrical configuration (Fig. 1(d)), the rotational effect must be considered.).

2) The rotational supersonic dispersion for H_2.

3) The use of the average energy of the thermal collisions will be replaced by the averaging procedure over the Maxwellian distribution etc.

The author is much indebted to Mr. T. Kishimoto for the helpful discussions about this work.

He is also thankful to Prof. M. Kotani for his deep interest in this paper.

References

1) C. Zener, Phys. Rev. **37** (1931), 556.
2) J. M. Jackson and N. F. Mott, Proc. Roy Soc. **A137** (1932), 703.
3) A. Van Itterbeek and P. Mariens, Physica **7** (1940), 909.
4) E. S. Stewart, Phys. Rev. **69** (1946), 632; J. E. Rhodes, Phys. Rev. **70** (1946), 932 (hydrogen); A. J. Zmuda, J. Acous. Soc. Amer. **23** (1951), 472 (nitrogen).
5) O. Nomoto, *Supersonics* (in Japanese) (1948) p. 46
6) L. Landau and E. Teller, Phys. ZS. Sowjet. **10** (1936), 34.
7) cf. ref. (2), Section 6, Eqs. (22), (23).
8) A. Eucken and E. Nümann, Z.S. Phys. Chem. **B36** (1937), 163.

Note added in proof:

Recently, we calculated the rotational dispersion of the supersonic wave in the hydrogen gas (see § 3). A satisfactory result was obtained. The detailed report will be published soon.

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Notes on the Decay of the Neutron, II*

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§ 5. Discussions I

If one considers only one pure interaction to describe the beta-decay,.....

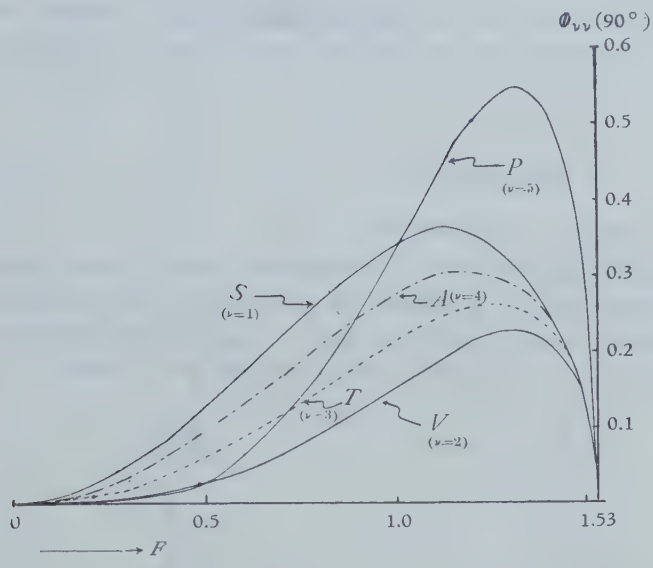
If experiments are actually carried out to determine the electron-proton angular correlation (§ 3) and the proton momentum spectrum (§ 4), it will be possible to determine which one of five interactions is responsible for the neutron decay process. Though these experiments may be considerably difficult to be carried out with present technique, it seems to us that they are not altogether impossible. So in this section we will summerize our theoretical predictions and give some discussions about our results. The spectra of emitted protons at angles $\varphi=90°$ and $\varphi=180°$ are shown in Figs. 2a and 2b. The curves of angular correlation for five interactions are given in Fig. 3.

First of all, the beta-spectrum for the P. interaction is markedly in disagreement with the experiment, as has been shown in Fig. 1. The proton momentum spectra at $\varphi=90°$ and $\varphi=180°$ show also peculiar behavior in the P. interaction. However the angular correlation $\Psi_{55}(\varphi)$ (3·8) for the P. interaction is rather similar to the V. interaction, and it is hardly distinguished from each other by the experiment. Now the question arises whether the experiments will be able to distinguish between first four interactions, S., V., T. and A. Its possibility just depends on the experimental accuracy, as has been often mentioned. (See Fig. 3.)

The proton spectra (§ 4) irrespective of the emitted angle of electrons are shown in Fig. 4. When comparing experiments with our theoretical results the situation is similar to that of the angular correlation.

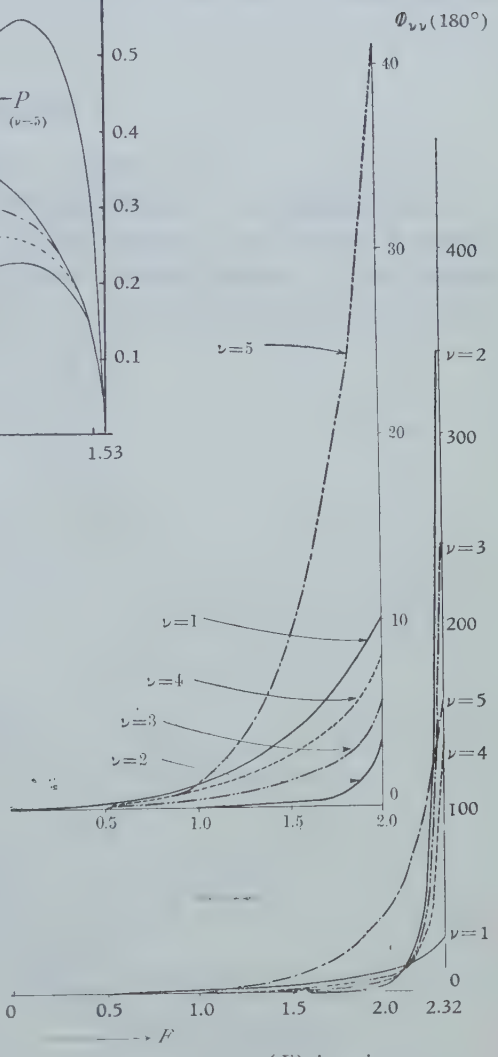
A clue for the choice of the type of interaction is given also by data of nuclear beta-decay processes. It is experimentally known that the $He^6 \rightarrow Li^6$ transition is an allowed

* Part I was published in Prog. Theor. Phys. 7 (1952), 469.



Proton momentum (F) in unit m.

Fig. 2a.



Proton momentum (F) in unit m.

Fig. 2b.

Fig. 2. Proton momentum spectra given by $(3\cdot1')$ for five interactions. Fig. 2a and 2b show spectra obtained at $\varphi=90°$ and $\varphi=180°$, respectively.

one and involves the change of the nuclear spin by unity ($\Delta I=1$).[15) 16)] The selection rules of the allowed transition given by the S. and V. interactions, known as Fermi's selection rules, do not permit any change of the spin units. The experimental result of He^6 certainly contradicts with these selection rules. Therefore, if one considers only one pure interaction to describe this result, the interaction needs to be either T. or A.; as has been pointed out by Gamow and Teller, the change of nuclear spin of one unit is permitted in these interactions even for the allowed transition. Unfortunately, the allowed electron spectrum does not give any unique information as regards the choice between

these alternatives, because both interactions give the same spectrum. But in principle the electron-proton correlation and the proton spectrum would be able to give a decision at this point.

§ 6. Discussions II

If one considers mixed interactions,.....

Our discussion on the experimental results above has been made under a rather special assumption that the true interaction must be determined by only one of five invariants. Recently there is a tendency among physicists to believe that a linear combination of five invariants is necessary rather than a pure interaction in the nuclear beta-decay process.[6] [7] [8]

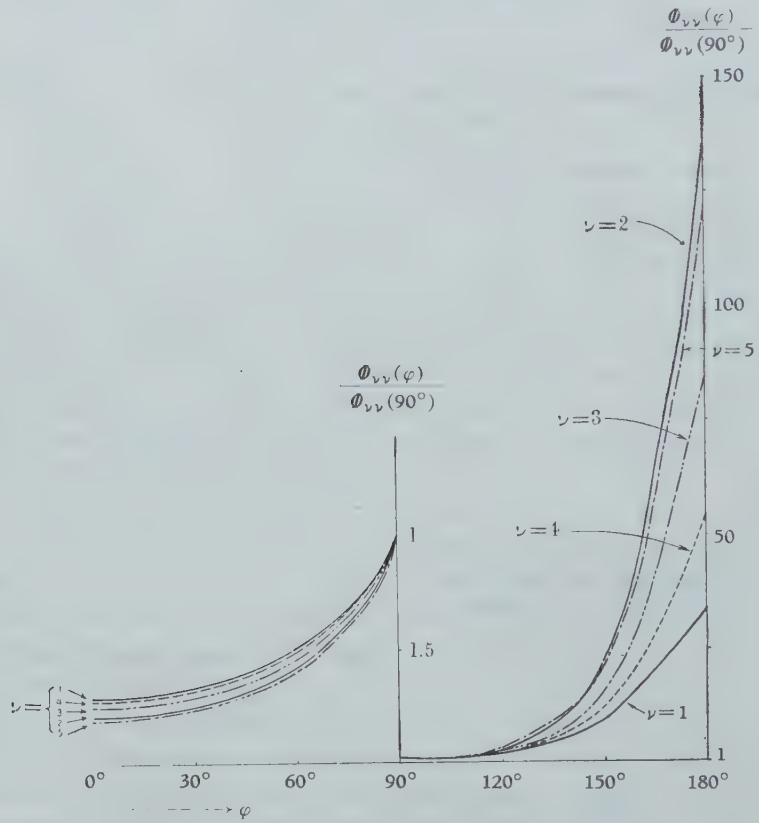


Fig. 3. Angular correlations of electrons and protons obtained from (3·7) in the cases of five interactions. These curves are normalized at $\varphi=90°$. For each interactions, the absolute values calculated at $\varphi=90°$ are given as follows;

$$\Phi_{11}(90°)=0.30, \quad \Phi_{22}(90°)=0.15,$$
$$\Phi_{33}(90°)=0.20, \quad \Phi_{44}(90°)=0.25$$

and

$$\Phi_{55}(90°)=0.33.$$

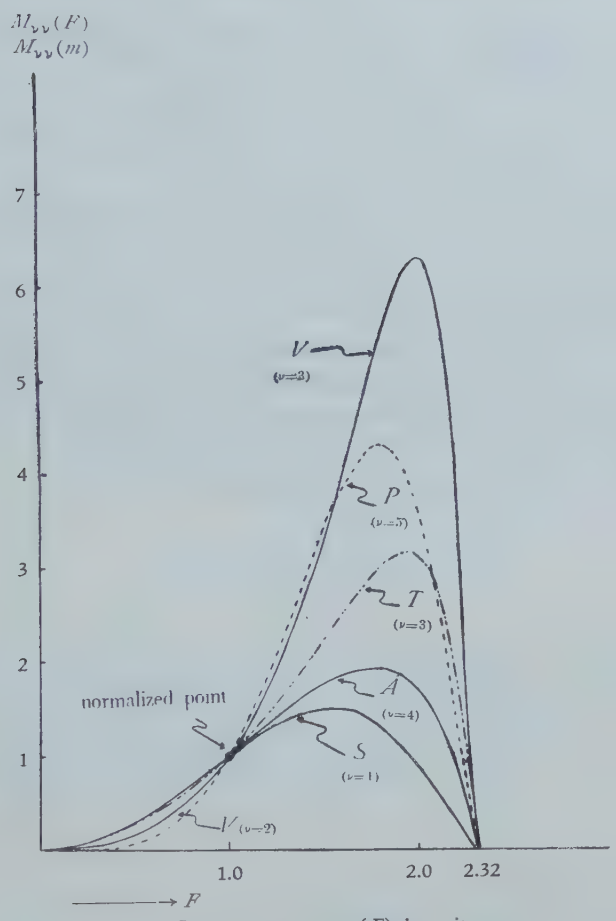


Fig. 4. Momentum spectra of emitted protons from (4·3) in the cases of five interactions. These curves are normalized at $F=m$. The absolute values calculated at $F=m$ for each interactions are given as follows;
$M_{11}(m)=0.90$, $M_{22}(m)=0.32$, $M_{33}(m)=0.51$,
$M_{44}(m)=0.70$ and $M_{55}(m)=0.90$.

For example, Petshek and Marshak[19] have studied how to explain the peculiar form of RaE spectrum by a linear combination of T. and P. In the case of the neutron decay, we can not say that the shape of allowed spectrum is completely in agreement with the experiments, if we take the fact seriously that the experimental results below 300 Kev. are smaller than the values theoretically expected under the assumption of the allowed transition. Of course, as has been described by Robson, these data have certainly considerable errors so that we can not believe these values as they are. But it is not meaningless to ask the question whether or not the present experimental data can be interpreted by the mixed interaction above, Robson's result in the lower energy region being taken seriously. The

effects of this linear combination were first calculated by Fierz[20] and later by Rozental[21] and by de Groot and Tolhoek.[17] Since no numerical results, especially no calculation for the neutron decay, have not yet been given, we shall discuss about the possibility of such mixtures. But we shall content ourselves only with studying the tendency, describing all four particles by the plane waves, as has been noted in § 2.

In this mixed interaction, the total transition probability is given by using $\sum_{\nu,\eta} G_\nu G_\eta S_{\nu\eta}$ in place of $G_\nu^2 S_{\nu\nu}$ in (2·3), where $\sum_{\nu\eta}$ means the sum over 1 to 5 corresponding to five interactions. $S_{\nu\eta}$'s are given in Table II and are identical with the results obtained by Fierz and Tolhoek and other authors.

In order to show the effects of the interference terms, it is enough to study only the cases in which two interactions are combined. The comparison between the theoretical and experimental beta-spectra will be done by the Kurie plot method. Namely, we shall plot the dependence of $(\sum_{\nu\eta} N(p)/p^2)^{1/2}$ on the electron energy (p_0), where $\sum_{\nu\eta} N(p)$ is obtained from the following expression corresponding to (2·4):

$$P=\frac{G_\nu^2 a_\nu^2}{2\pi^3}\int_0^{\varepsilon_2-m_2} dp \sum_{\nu\eta} N(p). \tag{5·1}$$

Table II. S_ν's in the linear combination of five interactions. The factors in the brackets indicate the order of magnitude of expressions. The thick letter means the term which changes the results by the interference effect; and 0 means that the cross correction term vanishes. $Sp_{\nu\eta}$ does not change when the suffixes ν and η are interchanged, e.g., $Sp_{12}=Sp_{21}$. $Sp_{\nu\nu}$'s have already been given in Table I.

	S.	V.	T.	A.	P.
S.	$\boldsymbol{Sp_{11}(1)}$				
V.	$\boldsymbol{Sp_{12}(1)}$	$\boldsymbol{Sp_{22}(1)}$			
T.	$Sp_{13}(m/M)$	$Sp_{23}(m/M)$	$\boldsymbol{Sp_{33}(1)}$		
A.	0	$Sp_{24}(m/M)$	$\boldsymbol{Sp_{34}(m/M)}$	$\boldsymbol{Sp_{44}(1)}$	
P.	0	0	$\boldsymbol{Sp_{35}(m/M)}$	$\boldsymbol{Sp_{45}(m/M)}$	$\boldsymbol{Sp_{55}(m^2/M^2)}$

$$\begin{aligned}
Sp_{12} &= \frac{1}{6}\cdot Sp_{34} = 16\, M_N m[(F\cdot q) - M_L\cdot p] \\
&\fallingdotseq -32\, M_N M_L m(\varepsilon - p_0), \\
Sp_{13} &= -Sp_{24} = -Sp_{35} = 32 M_N [q(F\cdot p) - p_0(F\cdot q)] \\
&\fallingdotseq 32 M_N(\varepsilon - p_0)[\varepsilon p_0 + m^2 - 2p_0^2 - p(\varepsilon - 2p_0)\cos\theta] \\
&\fallingdotseq 32 M_N[(\varepsilon - 2p_0)(\varepsilon^2 - m^2 - F^2)/2 + m^2(\varepsilon - p_0)], \\
Sp_{23} &= 6\cdot Sp_{45} = 96\, M_N m[(F\cdot q) + M_L q] \\
&\fallingdotseq -96\, M_N m(\varepsilon - p_0)[(\varepsilon - p_0) + p\cos\theta] \\
&\fallingdotseq -96\, M_N m\left[\varepsilon(\varepsilon - p_0) - \frac{(\varepsilon^2 - m^2 - F^2)}{2}\right].
\end{aligned}$$

In this expression the integrand is defined by

$$\sum_{\nu\eta} N(p) = N_{\nu\nu}(p) + 2g_{\nu\eta} N_{\nu\eta}(p) + g_{\nu\eta}^2 N_{\eta\eta}(p), \tag{5·2}$$

where

$$N_{\nu\eta}(p) = \frac{1}{\omega_\nu \omega_\eta} \int_{-1}^{1} d(\cos\theta) \frac{S p_{\nu\eta}}{64 M_N p_0 (\varepsilon - p_0) M_P}, \tag{5·3}$$

and $g_{\nu\eta}$'s are the mixing ratios of the ν and η interactions, which are defined by

$$g_{\nu\eta} = G_\eta \omega_\eta / G_\nu \omega_\nu . \tag{5·4}$$

We shall further discuss about the angular correlations and the proton-spectra. Now we shall give their expressions for various cases successively :

(i) For comparison's sake we first give the Kurie plot for the allowed transition, that is, the spectrum for the pure S., V., T. and A. interactions without mixing :

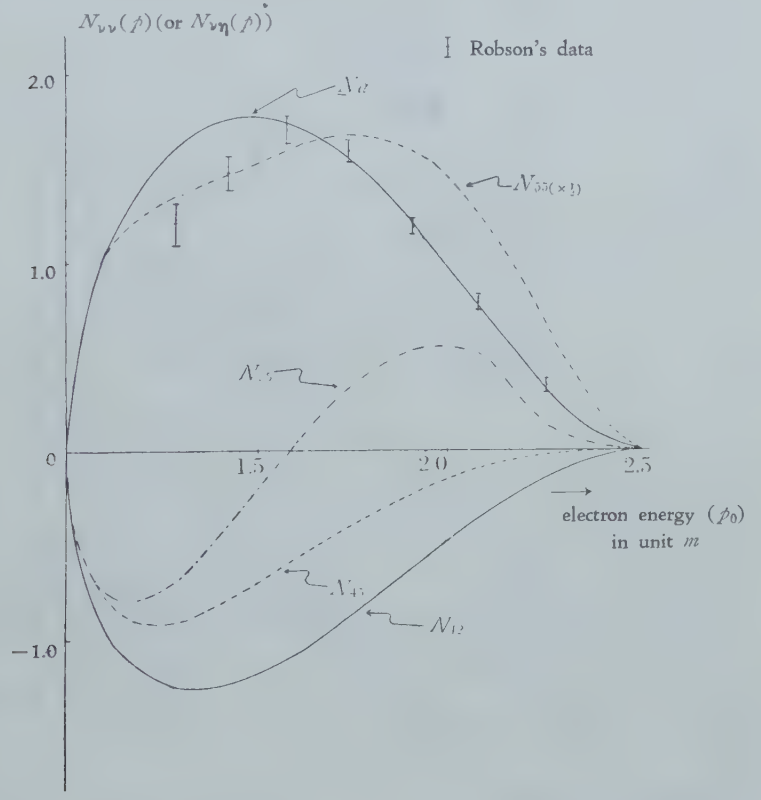


Fig. 5. Energy spectra of emitted electrons for the diagonal terms (N_{α} and N_{55}), which are obtained from the squares of five interactions, and their cross correction terms ($N_{\nu\eta}$). Their expressions are given as the following table;

$N_{\alpha}(p)$: (2·6) $N_{12}(p)$: (5·6)
$N_{55}(p)$: (2·7) $N_{35}(p)$: (5·17)
$N_{45}(p)$: (5·22).

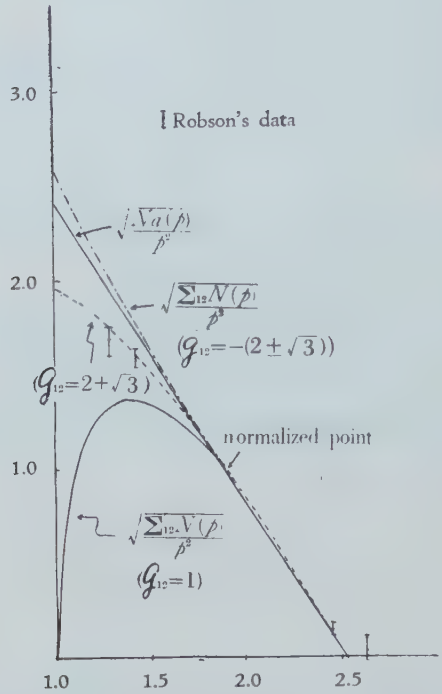


Fig. 6. Kurie plots in the case of linear combination; S. with V. These curves are normalized at $p=1.9\,m$. The expressions of $(N_a(p)/p^2)^{1/2}$ and $(\Sigma_{12}N(p)/p^2)^{1/2}$ are given by (5·5) and (5·7), respectively.

$$\sqrt{N_a(p)/p^2} \doteqdot (\varepsilon - p_0). \tag{5·5}$$

The straight line corresponding to this Kurie plot is shown in Fig. 6 with points showing the experimental data.

(ii) In the cases of interference of four interactions except P., the terms having the same order of magnitude as the allowed one are the terms arising from the interference between S. and V. and between T. and V. (See Table II). Thus we have the following two possibilities.

(iia) In the case where the V. interaction is mixed with S., the interference term (N_{12}) is obtained by inserting Sp_{12} into (5·3);

$$N_{12}(p) \doteqdot -(\varepsilon - p_0)^2 p^2 \cdot m/p_0 . \tag{5·6}$$

Therefore, we shall obtain the following expression corresponding to $(\sum_{\nu\eta}N(p)/p^2)^{1/2}$:

$$\sqrt{\frac{\sum_{12}N(p)}{p^2}} \doteqdot \{(1+g_{12}^2) - 2g_{12}(m/p_0)\}^{1/2}(\varepsilon - p_0). \tag{5·7}$$

We plot the graph of (5·6) in Fig. 5. The graph of (5·7) are plotted

in Fig. 6 for five values of g_{12}, in order to show how the spectrum changes with mixing ratio g_{12}. The values used for g_{12} are 1, $(2\pm\sqrt{3})$, and $-(2\pm\sqrt{3})$. We see that the curve for $g_{12}=(2\pm\sqrt{3})$ agrees with the experimental values obtained by Robson.

The angular correlation, in this mixture, is given by the following expression:

$$P=\frac{G_1^2 a_1^2}{2\pi^3}\int_{-1}^{1} d(\cos\varphi)\sum_{12}\Phi(\varphi), \tag{5·8}$$

where

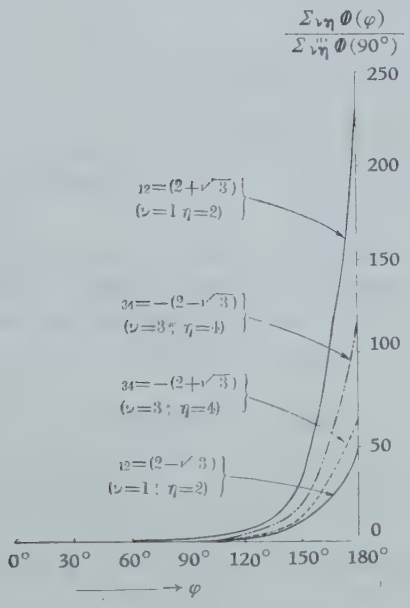


Fig. 7. Angular correlations of electrons and protons in the cases of linear combinations; S. with V., and T. with A. These curves are normalized at $\varphi=90°$. The expressions of $\Sigma_{12}\Phi(\varphi)$ and $\Sigma_{34}\Phi(\varphi)$ are given by (5·9) and (5·14), respectively.

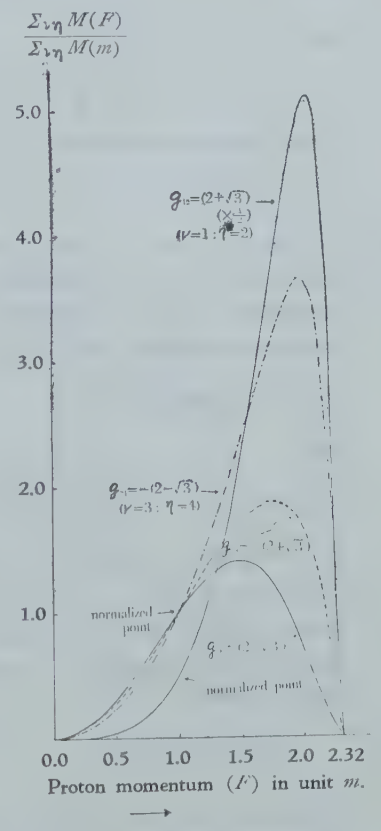


Fig. 8. Proton momentum spectra irrespective of the emitted angle in the cases of linear combinations; S. with V., and T. with A. These curves are normalized at $F=m$. The expressions of $\Sigma_{12}M(F)$ and $\Sigma_{34}M(F)$ are given by (5·12) and (5·15), respectively.

$$\sum_{12}\Phi(\varphi)\doteqdot\{I_b+g_{12}^2(2I_a-I_b)-2g_{12}I_d\}\,, \tag{5·9}$$

and

$$I_d=\frac{1}{2}\int_x^y dp_0(F^2p/\sqrt{D''})\,m(\varepsilon-p_0)\,. \tag{5·10}$$

These expressions correspond to (3·7) in § 3.

We shall further give the proton spectrum in this mixture. It is given by the following expression;

$$P=\frac{G_1^2a_1^2}{2\pi^3}\int_0^{\varepsilon_2-m_2} dF\sum_{12}M(F)\,, \tag{5·11}$$

where

$$\sum_{12}M(F)\doteqdot\{J_a+g_{12}^2(2J_a-J_b)-2g_{12}J_d\} \tag{5·12}$$

and

$$J_d=\frac{1}{4}\,(\varepsilon^2-F^2-m^2)^2F^2\varepsilon m/(\varepsilon^2-F^2)^2\,. \tag{5·13}$$

These expressions correspond to (4·3) in § 4. $\sum_{12}\Phi$ (5·9) and $\sum_{12}M$ (5·12) are, respectively, shown in Figs. 7 and 8 for two values of g_{12}, i.e. $g_{12}=(2\pm\sqrt{3})$.

(iib) In the case where T. and A. interactions are mixed, the expression N_{34} is the same with $(-N_{12})$. Therefore, we get the same beta-spectrum as (iia): one has simply to substitute g_{12} by $(-g_{34})$. But the expressions for the angular correlation and the proton-spectrum are different. We find that

$$\sum_{34}\Phi(\varphi)\doteqdot\left\{\frac{1}{3}[4I_a-I_b]+\frac{1}{3}g_{34}^2[2I_a+I_b]+2g_{34}I_d\right\}\,, \tag{5·14}$$

and

$$\sum_{34}M(F)\doteqdot\left\{\frac{1}{3}[4J_a-J_b]+\frac{1}{3}g_{34}^2[2J_a+J_b]+2g_{34}J_d\right\}\,. \tag{5·15}$$

$\sum_{34}\Phi$ (5·14) and $\sum_{34}M$ (5·15) are also respectively shown in Figs. 7 and 8 for two values of $g_{34}=-(2\pm\sqrt{3})$.

(iii) Before entering to the remaining mixtures, we give for comparison's sake the Kurie plot for the pure P interaction. From (2·7), the desired expression is easily found:

$$\sqrt{\frac{N_{55}(p)}{p^2}}\doteqdot\{p^2+(\varepsilon-p_0)^2-(2p^2(\varepsilon-p_0)/3p_0)\}^{1/2}(\varepsilon-p_0)/m\,. \tag{5·16}$$

The Kurie plot of (5·16) is shown in Fig. 9a. One can see clearly that it disagrees with the experiment.

(iv) Sp_{35} and Sp_{45} are apparently of the smaller order of magnitude by the factor (m/M) as compared with Sp's for the allowed transition. Sp_{55} given in Table II is still smaller, namely of the order of $(m/M)^2$. But these conclusions are based on the assumption that the P. coupling constant G_5 is of the same order of magnitude as the other G's. If it is assumed that G_5 has a suitable large value as that G_5a_5 becomes comparable with the other $G_\gamma a_\gamma$'s,

these interference terms are sufficiently large so that they can be respectively used in the mixed theories consisting of two interactions, of P. and T. and of P. and A.

(iva) In the case of mixing the P. interaction with T., the expressions corresponding to (5·6), (5·7), (5·9) and (5·12) are as follows:

$$N_{35}(p) \doteqdot \frac{-1}{\sqrt{3}} \frac{p_0(\varepsilon-p_0)-p^2}{mp_0}(\varepsilon-p_0)^2p^2, \tag{5·17}$$

$$\sqrt{\frac{Z_{35}N(p)}{p^2}} \doteqdot \left\{1+g_{35}\left(p^2+(\varepsilon-p_0)^2-\frac{2p^2(\varepsilon-p_0)}{3p_0}\right)\frac{1}{m^2} - \frac{2}{\sqrt{3}}g_{35}\frac{p_0(\varepsilon-p_0)-p^2}{mp_0}\right\}^{1/2}(\varepsilon-p_0), \tag{5·18}$$

$$\sum_{35}\Phi(\varphi) \doteqdot \left\{\frac{1}{3}[4I_a-I_b]+g_{35}^2I_c-\frac{2}{\sqrt{3}}g_{35}[I_a+I_e]\right\}, \tag{5·19}$$

$$\sum_{35}M(F) \doteqdot \left\{\frac{1}{3}[4J_a-J_b]+g_{35}^2J_e\right\}, \tag{5·20}$$

where

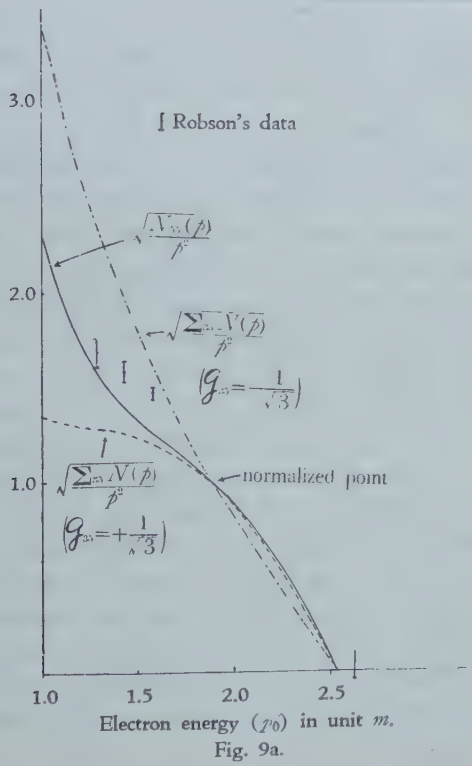


Fig. 9a.

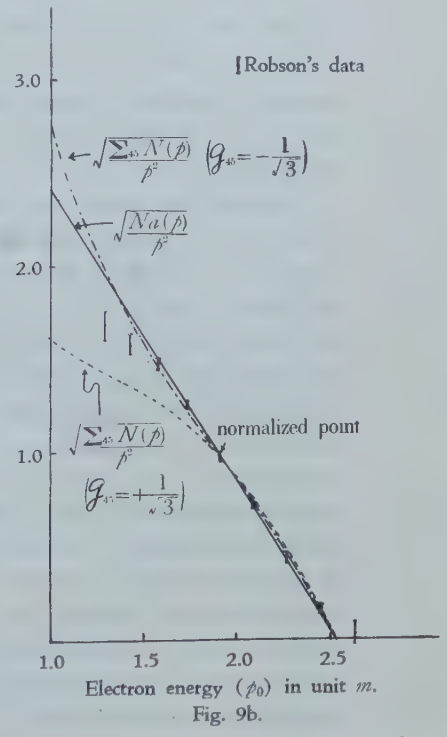


Fig. 9b.

Fig. 9. Kurie plots in the cases of linear combinations: Figs. 9a and 9b show plots for the combinations of T. with P. and A. with P., respectively. These curves are normalized at $p_0=1.9$ m. The expressions of $(N_{55}(p)/p^2)^{1/2}$, $(\Sigma_{35}N(p)/p^2)^{1/2}$ and $(\Sigma_{45}N(p)/p^2)^{1/2}$ are given by (5·16), (5·18) and (5·23), respectively.

$$I_e=\frac{1}{2}\int_x^y dp_0(F^2p/\sqrt{D''})(\varepsilon-2p_0)(\varepsilon^2-m^2-F^2)/2m^2. \quad (5\cdot21)$$

(ivb) In the case of mixture of A. and P. interactions, the corresponding expressions are,

$$N_{45}(p)=-\frac{1}{\sqrt{3}}\frac{\varepsilon-p_0}{p_0}(\varepsilon-p_0)^2p^2, \quad (5\cdot22)$$

$$\sqrt{\frac{\sum_{45}N(p)}{p^2}}=\left\{1+g_{45}^2\left(p^2+(\varepsilon-p_0)^2-\frac{2p^2(\varepsilon-p_0)}{3p_0}\right)\frac{1}{m^2}-\frac{2}{\sqrt{3}}g_{45}\frac{\varepsilon-p_0}{p_0}\right\}^{1/2}(\varepsilon-p_0), \quad (5\cdot23)$$

$$\sum_{45}\Phi(\varphi)=\left\{\frac{1}{3}[2I_a+I_b]+g_{45}^2I_c-\frac{2}{\sqrt{3}}g_{45}\left[\frac{\varepsilon}{m}I_a-I_b\right]\right\}, \quad (5\cdot24)$$

and

$$\sum_{45}M(F)=\left\{-\frac{1}{3}[2I_a+I_b]+g_{45}^2I_c-\frac{2}{\sqrt{3}}g_{45}\left[\frac{\varepsilon}{m}I_a-I_b\right]\right\}. \quad (5\cdot25)$$

Curves for (5·17), (5·18), (5·22) and (5·23) are plotted in Figs. 5 and 9. In Fig. 9 curves are drawn for rather large values of the parameters g_{35} and g_{45}; namely, we have taken $\pm(1/\sqrt{3})$ for both g's. If we take smaller values for both g's, the spectra resulting from these combinations approach the pure allowed one. We see in the figures that the observed data lie between the curve for the allowed spectrum and the curves with $g_{35}=g_{45}=+(1/\sqrt{3})$. This means that one will be able to account for the observed data by these mixtures if one takes the mixing ratios suitably. Here we will not enter to the precise determination of the mixing ratio, but give only the following remark. In the ordinary theory about the nuclear beta-decay processes, the first term arising from the P. interaction has been classified into the first forbidden transition and usually treated as a smaller effect compared with the allowed one. However, Petshek and Marshak,[19] who studied the *RaE* spectrum, found that the first term of the expansion of the P. interaction including the coupling constant is about thirteen times as large as the first forbidden one of the T. interaction. This may mean that the effect of the P. interaction is larger than usually considered, though, of course, we can not draw any definite conclusion before we have more accurate knowledge about the magnitude of the nuclear matrix elements for *RaE*. If the effect of the P. interaction is actually not small, it may be possible that the shape of the spectrum at the low energy region is accounted for by our mixtures.

Hitherto we have considered only the linear combinations of two interactions. The linear combinations of three or more invariants are, of course, not excluded, but the general

only the freedom of the theory. Also, it is possible to assume that the coupling constant has an imaginary value.[22] In order to obtain further information about such possibilities, more cases of nuclear beta-decay processes must be observed and investigated, and therefore we will not discuss them now. However, there is one important case to be considered. It is a permissible linear combination of S., A. and P. interactions, which was introduced by Critchfield and Wigner according to a symmetry principle.[23] In this case, both the cross correction terms of A. and P. with S. interaction vanish, and, as the result, the beta-spectrum obtained is the same with the case (ivb), including only the $S\beta_{15}$ terms. We will not, therefore, discuss this possibility in detail, though the curve for the angular correlation may be different from what has been given above. Besides the Critchfield-Wigner combination, there is a special combination of V. and T. interactions, which was proposed by De Groot and Tolhoek[17] according to their own symmetry principle. In this combination, the cross correction term is very small, so that this seems to be consistent, only when the experimental results confirm that the observed spectrum is actually in good agreement with the theoretical allowed spectrum.

Our above discussion about the linear combinations of some interactions has been founded on the assumption that below 300 Kev. the data measured by Robson are to be taken seriously. But Robson himself seems to believe that "in this region the known instrumental defects make the observed points inaccurate in their representation of true momentum spectrum" and that "above 300 Kev. their distribution is consistent with what is to be expected for an allowed transition." If the experimental Kurie plot is actually a straight line down to low energies indicating that the transition is allowed one, combinations (ii), i. e. the combinations of S. with V. and T. with A, must be excluded,[17] [20] while the combinations, which was not discussed above, i. e. combinations of S. with T., S. with A., V. with T. and V. with A., are all permissible.* It is because in these combinations the terms of interference either vanish or are smaller than the original (diagonal) terms, as has been indicated in Table II. If the P. coupling constant G_5 is of the same order of magnitude in comparison with the other, for example with G_1, $G_5 a_5$ is smaller than the other, e. g., $G_1 a_1$, and then the P. interaction does not give rise to any effect on the allowed transition so that any combinations including the P. interaction are all permissible.

Further experimental data will have to be used to decide whether the interaction is a pure one or a linear combination and whether the interference terms are necessary or not, if the combination is to be taken. In the case of the neutron decay process, more accurate information will be supplied by the experiments on the proton spectrum as well as those on the angular correlation of electrons and protons, besides the information supplied by a more accurate observation of the beta-spectrum.
feature of these combinations can be inferred by suitable consideration about the above discussed combinations of two interactions. Such combinations of many interactions increase

* According to the symmetry principle postulated by De Groot and Tolhoek, two combinations of S. with T. and V. with A. are also excluded.

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References

1) J. M. Robson, Phys. Rev. **78** (1950), 311; **83** (1951), 349. The preliminary results had reported by A. H. Snell et al., Phys. Rev. **74** (1948), 1217; **78** (1950), 310.
2) E. J. Konopinski, Rev. Mod. Phys. **15** (1943), 209.
3) H. A. Bethe and R. F. Bacher, Rev. Mod. Phys. **8** (1936), 82.
4) V. B. Berectetsky and I. Y. Pomeranchuk, J. Exp. Theor. Phys. U.S.S.R. **19** (1949), 756.
5) M. Taketani, S. Nakamura, K. Ono, and M. Umezawa, Prog. Theor. Phys. **6** (1951), 286.
6) Chien-Shiung Wu, Rev. Mod. Phys. **22** (1950), 386.
7) T. Kotani, S. Machida, S. Nakamura, H. Takebe, M. Umezawa and T. Yoshimura, Prog. Theor. Phys. **6** (1951), 1007.
8) T. Nakano, Y. Watanabe, S. Hanawa and T. Miyazima, Prog. Theor. Phys. **5** (1950), 1014.
9) S. C. Curren, J. Augus and A. L. Cockcroft, Phys. Rev. **76** (1949), 853.
10) D. R. Hamilton, Phys. Rev. **71** (1947), 456.
11) H. C. Wolf and G. E. Uhlenbeck, Phys. Rev. **46** (1934), 237.
12) E. Fermi, "*Elementary Particles*" (1951), Chap. Three, p. 42.
13) E. C. Nelson, Phys. Rev. **60** (1941), 830.
14) R. E. Marshak, Phys. Rev. **75** (1949), 513.
15) H. Brown and V. Perez-Mendez, Phys. Rev. **75** (1949), 1286; **77** (1950), 404.
16) J. S. Allen, H. R. Paneth and A. H. Morrish, Phys. Rev. **75** (1949), 570.
17) S. R. De Groot and H. A. Tolhoek, Physica **16** (1950), 456.
18) A. M. Smith, Phys. Rev. **82** (1951), 955.
19) A. G. Petshek and R. E. Marshak, Private communication to Prof. S. Tomonaga.
20) M. Fierz, Z. Phys. **104** (1937), 553.
21) S. Rozental, Danske Vid. Selsk. Wedd. **18** (1941), No. 7; **23** (1945), No. 11.
22) G. I. Trigg and E. Feenberg, Phys. Rev. **82** (1951), 982.
23) C. L. Critchfield and E. P. Wigner, Phys. Rev. **60** (1941), 412; **63** (1943), 417.

Note added in proof: Erratum In the preceding paper (Part I) of same authors, $x=0$ on page 477 (first and eighth lines) should be replaced with $x=\infty$.

Letters to the Editor

Non-Local Theory of Nucleon-Meson Field

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June 10, 1952

The pseudo-vector interaction of nucleons with paeudo-scalar mesons seems to be the most hopeful one in the theory of nucleon and π-meson system, but for this type of interactions the renormalization procedure cannot be applied in the present formalism of the theory and moreover the perturbation method cannot give a good approximation in high energy regions. When we attempt to remove the divergences by means of the renormalization method, we are obliged to introduce infinite number of counter interactions having successively higher order derivatives of field variables. The renormalized interactions thus obtained can be interpreted as non-local one[1], while the theory of non-local interactions may be translated into the theory of non-local particles as we have conjectured in the recent paper[2]. Now, we assume that both nucleons and p.s. mesons are non-local particles. Then we can show that the S-matrix is divergence-free and its perturbation expansion gives a good approximation.

We define the wave function Ψ for nucleons as follows:

$$\Psi_\alpha(X-x,x)=\bar{\xi}_{\alpha\rho}(X-x)\psi_\rho(x),$$

$$\Psi_\beta(X-x,x)=\bar{\psi}_\sigma(x)\bar{\xi}^{+}_{\sigma\beta}(X-x), \quad (1)$$

$$\begin{cases}[\gamma_\mu\cdot\partial/\partial x_\mu+\mu_0]\psi(x)=0,\\ [\bar{\gamma}_\mu\cdot\partial/\partial x_\mu-\mu_0]\bar{\psi}(x)=0,\end{cases}$$

$$\gamma\{\mu\gamma\nu\}=2\delta_{\mu\nu}, \quad (2)$$

$$[\beta_\mu\cdot\partial/\partial(X-x)_\mu+\mu]\bar{\xi}(X-x)$$
$$=(\mu^2-\mu_0^2)^{1/2}\ \delta^4(X-x), \quad (3)$$

$$\beta\{\mu,\beta\nu\}=2\delta_{\mu\nu}\quad[\gamma,\ \beta]=0 \quad (4)$$

where ξ is a matrix which describes something about the inner structure of the nucleon. Owing to (4) both γ and β are 16—16 matrices, and accordingly Ψ has 16 components. We can verify the Lorentz-invariant property of this nucleon field.

Representing the inner structure of the meson by a scalar function $\zeta(x)$, the wave function Φ is defined as follows:

$$\Phi^{(j)}(X-x,x)=\zeta(X-x)\phi^{(j)}(x), \quad (5)$$

$$[\partial^2/\partial x_\mu^2-\varkappa_0^2]\phi^{(j)}(x)=0,$$

$$[\partial^2/\partial(X-x)_\mu^2-\varkappa^2]^{1/2}\cdot\zeta(X-x)$$
$$=i(\varkappa^2-\varkappa_0^2)^{1,2}\cdot\delta^4(X-x). \quad (6)$$

In defining the S-matrix, we require that (a) it is the unitary matrix and that (b) it must become the traditional S-matrix of the local theory in low energy regions. (In the low energy regions, $p^2\langle\langle\mu^2$ $(\mu>\mu_0)$ and $k^2\langle\langle\varkappa^2(\varkappa>\varkappa_0)$, one sees $\xi_{\alpha\beta}(r)\to\delta_{\alpha\beta}\cdot\delta^4(r)$ and $\zeta(r)\to\delta^4(r)$.) Moreover, we notice the fact that the pseudo-vector interaction

$$\bar{I}=\frac{ig^{(j)}}{\varkappa_0}\int\cdots\int(dX)\,(dx)\,(d\bar{x})\,(dy)\cdot$$
$$[\Psi(X-\bar{x},\bar{x})\gamma_5\gamma_\mu\tau^{(j)}\Psi(X-x,x)\cdot$$
$$\partial\Phi^{(j)}(X-y,y)/\partial X_\mu] \quad (7)$$

may be considered as the local interaction containing higher order derivatives of the conventional local fields $\bar{\psi}(x)$, $\psi(x)$ and $\phi^{(j)}(x)$. Then, taking the investigations of Matthews[3] and Koba[4] into account, we can define the S-matrix by

$$S[\infty,-\infty]=\sum_{n=0}^{\infty}\left(\frac{-i}{\hbar c}\right)^n\left(\frac{1}{n!}\right)\int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty}[dx].$$

$$[d\bar{x}][dx][dy]\cdot P\begin{pmatrix}x\\ \bar{x}\\ y\end{pmatrix}(I(X_1,\bar{x}_1,x_1,y_1),\cdots$$

$$\cdots\cdots I(X_n,\bar{x}_n,x_n,y_n)). \quad (8)$$

The operators representing internal lines of nucleons and mesons are given by

$$\iint(d\bar{x})\,(dx')\left\langle P\begin{pmatrix}\bar{x}\\ x'\end{pmatrix}(\bar{\Psi}_\alpha(X-\bar{x},\bar{x}),\right.$$
$$\left.\Psi_\beta(X'-x',x'))\right\rangle_0=\frac{1}{2}\varepsilon(x-x')\cdot$$
$$S^{(c)}_{\beta\alpha}(x'-x), \quad (9)$$

$$S^{(c)}_{\beta\alpha}(x) = -\frac{2i(\mu^2-\mu_0^2)}{(2\upsilon)^4} \lim_{\epsilon\to+0} \int(dp)\, e^{ipX}\ (i\gamma p-\mu_0)_{\alpha\beta}/(p^2+\mu_0^2-i\epsilon)\cdot (p^2+\mu^2-i\epsilon)$$

and

$$\iint(dy)(dy')\left\langle P\begin{pmatrix} y \\ y' \end{pmatrix}(\Phi^{(i)}(X-y,y),\ \Phi^{(j)}(X'-y',y'))\right\rangle_0 = \frac{1}{2}\hbar c\,\delta_{ij}\cdot \Delta^{(c)}_m(X-X'), \quad (10)$$

$$\Delta^{(c)}_m(X) = -\frac{2i(\varkappa^2-\varkappa_0^2)}{(2\pi)^4} \lim_{\epsilon\to+0} \int(dk)\, e^{ikX}/(k^2+\varkappa_0^2-i\epsilon)\cdot (k^2+\varkappa^2-i\epsilon)$$

respectively, where the definitions of P and $\varepsilon(x)$ are the same as that of Koba[4]

Thus obtained S matrix is entirely divergence-free, since the convergence condition for an arbitrary integral $M(E_n, E_m)$ is given by

$$\frac{1}{2}E_n + E_m + 2n - 4 \geq 1,$$
$$(E_m = \sum_j E^{(j)}_m,\quad n = \sum_j n_j). \quad (11)$$

When the wave length of a particle participating in an arbitrary phenomenon is λ, we can show the following relation

$$|S^{(n+1)}|/|S^{(n)}| \approx \left(\frac{\lambda}{l_0}\right)^2 < 1,$$
$$\frac{1}{l_0^2} = \left(\frac{\varrho^2}{\hbar c}\right)^{1/2}\frac{\varkappa\mu^2}{\varkappa_0} \quad (12)$$

in high energy regions. Accordingly the perturbation-expansion method of the S-matrix gives a sufficiently good approximation.

The detailed account will be published in the later issue of this journal. I wish to express my sincere thanks to Prof. Y. Mimura for his kind interest in this work, and also to Prof. K. Sakuma, Mr. T. Ouchi and Mr. Y. Miyachi for their useful discussions.

1) A. Petermann and E.C.G. Stueckerberg, Phys. Rev. **82** (1951),548; Helv. Phys. Acta **24** (1951), 317.
S. Sakata, H. Umezawa and S. Kamefuchi, Phys. Rev. **84** (1951), 154.
2) N. Shono and N. Oda, Prog. Theor. Phys. (to be published).
3) P. T. Matthews, Phys. Rev. **76** (1949), 684; Phil. Mag. **41** (1950), 185.
4) Z. Koba, Prog. Theor. Phys. **5** (1950), 696.

The Transition Effect of the Star Production

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The frequency of cosmic ray stars produced under various thickness of absorber has been given by several authors[1-4]. The observed transition curve[1] has a maximum near 1.2cm Pb thickness and its magnitude is larger than that at 0 cm thickness by about 30%.

Most part of the stars may be produced by the nucleon component in cosmic rays, whose frequency decreases gradually with the thickness of absorber according to its relatively long mean free path (—310 g/cm^2 for Pb). Therefore, the components, which give the maximum of transition curve under the thin absorber, may be considered to de different from the nucleon component. As is easily seen, one of them seems to be the photon component, while the slow proton, which is relatively abundant in the high altitude, and the backward scattering of nucleon in the absorber would also play some role. These three effects have been treated in this note.

(I) The effect of photons:

Schopper et al.[1] have already pointed out the contribution of the photon for the star production. Some remarks should be given for the value of the cross section of the star production by the photon. Most part of the cascade photons which give the maximum intensity near 1cm Pb belongs to rather low energy region ($\lesssim$100 Mev), where it is impossible for photons to produce the π-meson in the nuclear interaction. From such view-point, the author*) has estimated the effect of photons for the star production, according to the dipole interaction[5] of the photon with the nucleus, and found that its contribution is small by a factor in order to explain the observed

maximum. However, it has been pointed out[6] that the virtual π-meson's effect in nucleus (exchange effect) is considerable even in the energy below the threshold for the π-meson production. The result taken account of this effect is presented in Fig. 1 and the agreement with the experiment is successful, though the Rossi-Greisen's shower theory has been used[7]. Therefore, we have concluded that the maximum near ~1 cm Pb of the transition curve of the star production is almost due to the cascade photons.

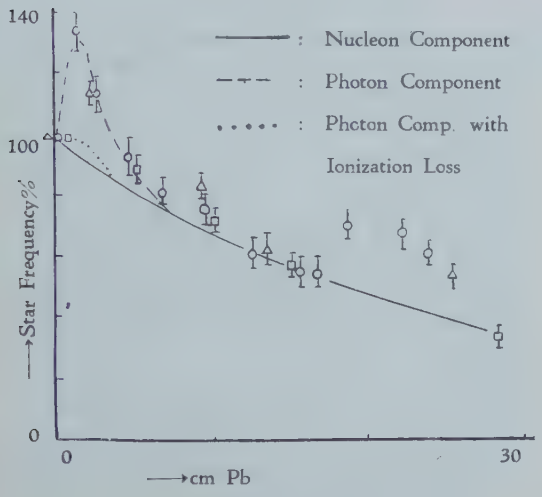

Fig. 1. The relative number of the cosmic ray stars *vs* the thickness of lead.
○: Schopper et al.
△: Bernardini et al.
□: George and Jason.

(2) The effect of slow protons:

The slow proton incident on the absorber may be partly stopped by its ionization loss before a nuclear interaction occurs and its contribution to the star production may be concentrated on the thin absorber. If one know the incident proton spectrum in low energies, one can calculate this contribution. Let $N(p_i)$ be the momentum spectrum of proton derived from the data of Mylroi-Wilson[8], where the incident momentum p_i is related to the momentum p_f at the thickness x of the absorber as $p_i = p_i(p_f, x)$. The average prong number $\langle n\ (p_f)\rangle$ of the star struck by the proton with momentum p_f is calculated from the data of Camerini et al[9]. Assuming the Poisson's distribution, we obtain the probability $S(p_f, n)$ of n prong numbers emitted by a proton (momentum p_f) when it collides with the nuclei. The frequency $I(n, x)$ of n pronged stars at the thickness x is given by,

$$I(n,x) = \int_0^\infty N[p_i(p_f,x)] \cdot S(p_f, n) \frac{\partial p_i}{\partial p_f} dp_f \cdot \sigma(\text{star}).$$

We have neglected the secondary nuclear effects, because we are only interested in the low energy proton. $\sum_{n\geq 2} I(n, x)$ is presented in Fig. 1. The slow proton makes the decrease of frequency less steep in the small thickness and this situation may not be changed under other absorbers, since the coefficient of ionization loss of them does not widely differ from that of lead in low energies.

(3) The effect of backward scattering:

In the star production, the high energy nucleon may produce the secondary nuclear components which are also capable to cause the star. The secondaries scattered backwards contribute to the star formation in the thin absorber. On account of the scarcity of detailed knowledge, we only give some crude estimation of this effect. Assuming one dimensional treatment, we take forward and backward scattering fraction as a and b respectively, and the mean free path of the nuclear collision as $1/\lambda$. Then the star production at x is given by,

$$a\int_0^x \exp\{-\lambda(x-x')\}\exp(-\lambda x')dx' + b\int_x^\infty \exp\{-\lambda(x'-x)\}\exp(-\lambda x')dx',$$

where the tertiary effect is neglected. Using the data of Bernardini et al.[10] for a and b, the maximum appears at the thickness of about 11cm Pb, where the increase of the frequency amounts to about 17%. However, because of our crude treatment, the obtained result should be thought as qualitative.

In this note, we have mainly analysed the first maximum of the transition curve. The second maximum (at near 20cm Pb) may be considered as the secondary nuclear effects which are responsible for the second maximum of the penetrating shower.

The author would like to express his gratitude to Prof. S. Sakata for his interest in this work and to Mr. S. Ogawa for his valuable discussions. He is also indebted to the Yukawa Yomiuri Fellowship for the financial aid.

1) E. Schopper, H. H. Höcker u. E. Rössle, ZS. f. Naturf. **6a** (1951), 603.
2) G. Bernardini, G. Cortini and A. Manfredini,

Phys. Rev. **79** (1950), 952.
3) G. Belliboni, L. Fabbrichesi, L. de Marco et M. Merlin, Nuovo Cim. **8** (1951), 374
4) M. M Shapiro, B. Stiller, M. Birnbaum and F. W. O'Dell, Phys. Rev. **83** (1951), 455.
*) H. Komori, Tokyo Meeting of Jap. Phys. Soc. Oct. 1951.
5) J. S Levinger, Phys Rev. **84** (1951), 43.
6) Y. Nagahara and J. Fujimura, Prog. Theor. Phys in press.
7) J. Nishimura and K Ida, Prog Theor Phys. **6** (1951), 905.
8) M. G. Mylroi and J. G Wilson, Proc. Phys. Soc. **A64** (1951), 404.
9) U. Camerini, J. H. Davies, P. H. Fowler, C. Franzinetti, H. Muirhead, W. O. Lock, D. H. Perkins and G. Yektieli, Phil. Mag. **42**(1951), 1241.
10) G. Bernardini, E. T. Booth, L. Lederman and J. Tinlot, Phys. Rev. **82** (1951), 105.

The Asymptotic Expression for the Structure Function of Interacting Particles

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It is desirable that we calculate the structure function of interacting particles without using any approximation except the fact that the number of particles is extremely large.

Denoting by $\Omega_N(E_p)$ the volume of the set of points the potential energy corresponding to which is less than E_p in the configurational space of N particles, the problem to find the asymptotic expression of $\Omega_N(E_p)$ as $N\to\infty$ can be partly solved as follows.

We assume that

$$E_p=\sum_{i>j}^{i=N}\sum_{j=1}^{j=N-1} u(r_{ij})$$

where $u(r_{ij})$ is the potential energy of the pair of particles i and j as a function of their distance apart r_{ij},

$$u(r_{ij})=0 \quad \text{for} \quad r_{ij}\geq r_1$$

and for $r_{ij}<r_1$

either Case (I)

$$|u(r_{ij})|<A \quad \text{for} \quad 0=r_0<r_{ij},$$

or Case (II)

$$|u(r_{ij})|<A \quad \text{for} \quad r_0\leq r_{ij}<r_1,$$

$$u(r_{ij})=\infty \quad \text{for} \quad r_{ij}<r_0,$$

where r_1, r_0, and A are constants.

Writing

$$\Omega_N(E_p)=g(v)F_N(E_p)$$

where v is the volume of the container and $g(v)$ is the volume of the cofigurational space accessible by the system (in the case (I) $g=v^N$), $F_N(E_p)$ may be interpreted as the distribution function of E_p, and our problem reduces to that of the theory of probability.

Introducing the new variable $\chi_N=E_p/\sqrt{N}$ and suitably changing the origin of the energy, we find that the every moment of χ_N whose distribution function is $G_N(\chi_N)=F_N(E_p)$ tends to that of the Gaussian distribution as $N\to\infty$ fixing the density $\rho=N/v$.

It can be proved that the Taylor expansion of the characteristc function of $G_N(\chi_N)$ converges uniformly with respect to N for fixed ρ. Accordingly, the characteristic function of $G_N(\chi_N)$ tends to that of Gauss, which results in

$$F_N(E_p)\simeq 1/\sqrt{2\pi N\mu_2}\times$$

$$\int_{-\infty}^{E_p-2\pi\rho N\int_{r_0}^{\infty}u(r)r^2dr} \exp\left(-z^2/N\mu_2\right)dz$$

where

$$\mu_2=2\pi\rho\int_{r_0}^{\infty}u^2(r)r^2dr.$$

This is rigorous so long as E_p is arbitrarily fixed as $N\to\infty$. But if we want to make use of this to the statistical mechanics (for example, the expression for entropy), E_p must be increased proportionally to N. This fact seems to make the direct application of this result to the statistical mechanics in the lower temperature range very doubtful. Under the assumption (I) however, it is found that our method gives the correct value to the free energy in the limit $\sqrt{\rho}/kT\to 0$, which may be compared with the well known Mayer's theory of imperfect gas where the contribution from higher irreducible integrals becomes zero in the limit $\rho/kT\to 0$.

The author is indebted to Professor M. Kotani, Assistant Professor T. Yamamoto, and Mr. E. Teramoto for the valuable discussions.

Radiative Correction to β-Decay Matrix Element

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June 26, 1952

Recently, the problem of field correction to the β decay matrix element has been discussed by several authors.[1)2)] As is well known, the renormalization theory is applicable for theories with 1st kind interactions only, but it is no more so for those with 2nd kind interactions.[3)] Hence, for the Fermi type interaction, belonging to the latter, there appears the infinite number of divergences, being not renormalizable.[3)4)] The electromagnetic or meson fields, however, can interact with spinor fields via the 1st kind interaction and so there arises the question whether the divergences are renormalizable or not, which appear in the higher order corrections to the Fermi-type interaction. The radiative correction was already discussed by Nakano et al[1)]. in the lowest order approximation, but here we shall consider it more generally, (higher order corrections). The answer is in the affimative.

The interaction is

$$H=H_1+H_2,$$

$$H_1=\sum_i g_i\bar{\Psi}(x)\bar{\varphi}(x)(\beta B)_i\psi(x)\times\Psi(x)+\text{conj.}, \qquad (1)$$

$$H_2=-ieA_\mu(\bar{\Psi}(x)\Gamma_\mu\Psi(x)-\bar{\psi}(x)\gamma_\mu\psi(x)),$$

where the notations are the same as in reference 1 and subscript i indicates the coupling type.

As mentioned above, our considerations are confined to the S matrix element with four external fermion lines of the order ge^{2n}. In general, an irreducible graph is divergent, which satisfies the following condition

$$3/2\cdot E_f+E_b+\sum n_l K_l<5, \qquad (2)$$

where E_f and E_b are numbers of external lines of fermion and boson respectively, and n_l the number of vertices due to the interaction H_l with the characteristic constant K_l[3)]. In our case, the left hand side becomes 4 because $E_f=4$, $E_b=0$, $K_1=-2$, $K_2=0$ and $n_1=1$. Thus, the order of divergence is logarithmic. Suppose that in a given reducible graph all the internal divergences, separated by the usual prescription, have already been removed. From the familiar arguments in renormalization theory the order of divergence of the final integration for this graph is again logarithmic. Its matrix element is written in the form

$$M=\sum_i g_i\bar{\Psi}(x)\bar{\varphi}(x)(\beta B)_i F(\sigma)\psi(x)\Psi(x)+\text{conj.}, \qquad (3)$$

where F is a Lorentz scalar. The divergent part F_{div} of F is merely a constant (matrix) which does not involve the derivatives operating on ψ or Ψ, for the order of divergence is logarithmic. Hence, F_{div} is to be of the form

$$F_{div}=\sum_j G_j(\beta B)_j, \qquad (4)$$

where G_j's are divergent constants. Insertion of (4) in (3) gives the diverging part M_{div} of M:

$$M_{div}=\sum_i \mathfrak{g}_i\bar{\Psi}(x)\bar{\varphi}(x)(\beta B)_i\psi(x)\Psi(x)+\text{conj.}, \qquad (5)$$

where $\mathfrak{g}_i$ is given by

$$\sum_{ij} g_i(\beta B)_i G_j(\beta B)_j=\sum_i \mathfrak{g}_i(\beta B)_i. \qquad (6)$$

Since each term in (5) is of the same form as the term of the primary interaction H_1, we can remove these divergences either by renormalizing the coupling constants g_i's or by subtracting them by means of counter terms with divergent coupling constants.

As the divergences coming from β vertex can be removed in this way and those arising from internal lines and electromagnetics can be renormalized in the same way as in quantum electrodynamics,[5)] we can conclude in general that all the divergences are completely removed by the method of renormalization.

Nakano et al[1)]. have shown in the lowest order a possibility that without use of renormalization divergent terms M_{div} are compensated by appropriately choosing the coupling constants g_i's of primary interaction H_1. After some calculation of sedinions, we have obtained the necessary and sufficient

condition for such compensation to be possible. While the lowest order result satisfies this condition, it seems almost improbable that this condition holds in each order of approximation. Furthermore, even if it holds a single set of values of g_i's may be impossible to compensate the divergent terms in every order.

It is an interesting fact that as far as the specific matrix elements are concerned, the divergences are removed by renormalization even if the 2nd kind interactions are participating. It may also be of some interest to make further investigation as to the effect of extracted finite parts of radiative corrections on selection rules and energy spectra.

The author expresses his thanks to Prof. S. Sakata and Mr. H. Umezawa for their kind interest and valuable discussions.

1) Nakano, Watanabe, Hanawa and Miyazima, Prog. Theor. Phys. **5** (1950), 1014.
2) Kotani, Machida, Nakamura, Takebe, Umezawa and Yoshimura, ibid. **6** (1951), 1007.
3) Sakata, Umezawa and Kamefuchi, ibid. **7** (1952) 377, 551.
4) Kamefuchi, ibid. **6** (1951), 175.
5) Dyson, Phys. Rev. **75** (1949), 1736.

The State of Solid Methane as inferred from Nuclear Magnetic Resonance

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Proton magnetic resonance data[1] in solid methane were analyzed by using the one parameter theory[2] and the perturbation method. Assuming a single molecule as a unit of reorientation we obtained from the spin-lattice relaxation time the result shown in Fig. 1, where $\log_{10}\tau_c$ is plotted against reciprocal tem perature. τ_c decreases with increasing temperature and rather sudden alterations of the dominant mechanism for spin-lattice relaxation exist at about $20°K$ (λ-transition), $65°K$ (anomaly not yet detected by thermal measurements) and $90°K$ (melting point). The linear character revealed in the plot suggests that the dominant mechanism above $20°K$ is a thermal jumping or tunnelling over some fixed pass, the height of which is estimated

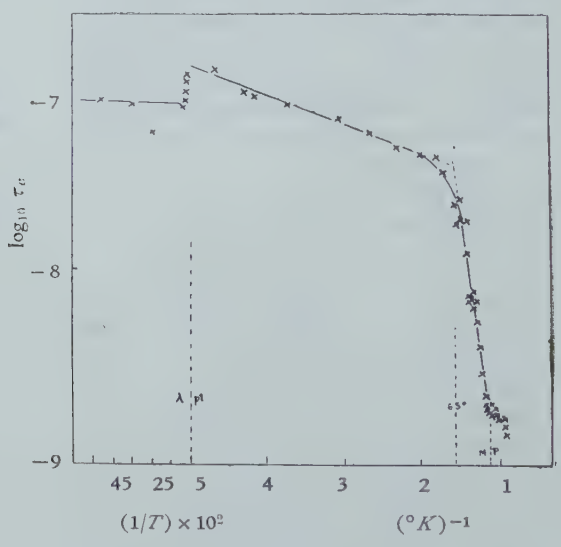

Fig. 1 Characteristic time τ_c determined from spin-lattice relaxation. $\log_{10}\tau_c$ is plotted against reciprocal temperature.

from the plot as 68 cal/mole or $20<T<65°K$ and 1380 cal/mole for $65<T<90°K$. A tentative picture we have in mind is as follows. Molecules rotate correlatedly and in gear with each other below $65°K$, while above $65°K$ they rotate more freely and independently and collide with each other less frequently but more violently than in the former case. Below $20°K$ τ_c seems almost independent of temperature, which suggests that each molecule is confined to its lowest group of levels, the width of which is small compared with kT. However, transition may occur inside this lowest group which corresponds to a tunnelling or flopping of each molecule among a number of equivalent potential minima. This is the reason why we have $\tau_c \sim 10^{-7}$ sec instead of $\tau_c \to \infty$ (as expected in the rigid lattice). Another support of this idea is given by the fact that the observed line width is only about one half that of a fixed molecule.

Spin spin relaxation time is estimated by taking the adiabatic second moment of the absorption line, and is given by $(T_2')^{-1}=[3K_1\pi^{-1}\tan^{-1}(2\pi\nu_m\tau_c)]^{1/2}$, where ν_m is the maximum frequency of the molecular modes of motion which contribute to the observable local field. Two cases should be discriminated concerning ν_m possibly in relation to the observing frequency. (1) When τ_c is long, the quasi-static or kinematical picture is observed. Local field due to magnetic interactions causes an adiabatic accerelation or decerelation of the main precession, which should be detected as a shift or width of the resonance line. However, the effect of those modes which are higher than the applied frequency ν_0 is averged out over one cycle of the radiofrequency and cannot be detected. In this case we should take $\nu_m=\nu_0$. Assuming $d=0.162$, the line width is fairly reproduced when $T<50°K$ including its local characteristics (2) When τ_c becomes short, however, marked discrepancy appears between the kinematical picture and the observation (at about $50°K$, where there is no anomaly in τ_c). We can include this case too in the one parameter theory if we adopt a cooperative or correlated limit for ν_m, the procedure of Bloembergen *et al.* being one such example. Empirically we may take $\nu_m=e/(T_2')^n$. A good reproduction of the line width is obtained if we take $e=0.184$ and $n=1.44$ above $50°K$. This set of values is satisfactory over two regions for which the dominant mechanisms of relaxation are different. (Fig. 2)

Finally the method of perturbation was applied to calculate the entire shape of the absorption line below $20°K$. Assuming F $\bar{4}$3m arrangement of molecules (which is supported by the entropy consideration[3]) and taking account of the spin-rotational selective combination, we obtained the results shown in Fig. 3, which is in close agreement with the experimental data observed[4] at $1.9°K$ and $4.2°K$. Also

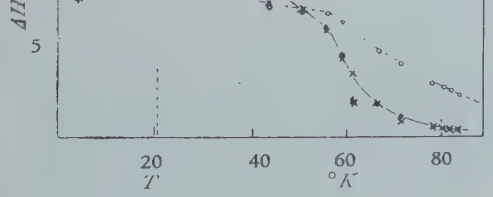

Fig. 2.
Half-value width $\Delta H_{1/2}$ calculated from spin-lattice relaxation. (The open circles and the broken line represent the values calculated under the assumption of a quasi-static local field. The closed circles and the full line represent the values calculated under the assumbtion of a dynamic local field. ×'s represent the observed values.)

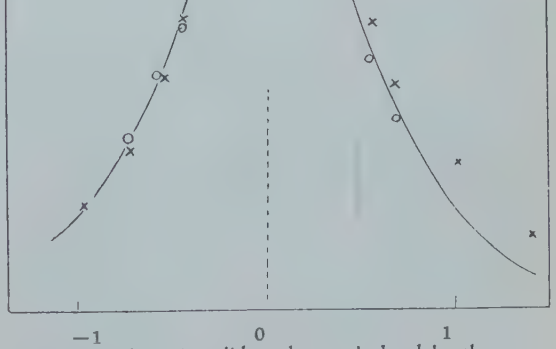

Fig. 3. Line shape in solid methane calculated by the perturbation theory. (×'s represent the observed values at $4.2°K$, and ○'s represent the observed values at $1.9°K$. The scale unit is 7.472 gauss.)

this result confirms our picture which is stated above. A similar analysis can be applied to the case of solid hydrogen.[5] The details will be published soon.

1) Thomas, Alpert and Torrey, J. Chem. Phys. **18** (1950), 1511.
2) Bloembergen, Purcell and Pound, Phys. Rev. **73** (1948), 679.
3) T. Nagamiya, Prog. Theor. Phys. **6** (1951), 702.
4) N. L. Alpert, Private communication.
5) Hatton and Rollin, Proc. Roy. Soc. (London) **199** (1949), 222.

An Interpretation of the Meso-disintegration of the Deuteron in Terms of the Strong Coupling Meson Theory

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The experiments by Durbin et al.[1] of the absorption of positive pions by deuterons reveald the predominantly $\cos^2\theta$ angular distribution of protons and the rapid increase of total cross section with incident energy. Both of these facts are in definite disagreement with calculations based on the weak coupling approximation[2], which yields the isotropic angular distribution and decrease of the cross section with energy. Chew et al.[3] proposed a mechanism to acconnt for the correct angular distribution, yet they were unable to account for the steep energy dependence of the cross section[4].

In this letter we shall briefly describe the results obtained from the pseudoscalar meson theory with strong coupling. The strong coupling theoretical treatment for two-nucleon system was carried out in the adiabatic approximation. The derived hamiltonian consists of, asides the kinetic energies of two-nucleons and free meson energy, the nuclear potential as well as the isobar energies and interactions with unbound mesons of each nucleon. The latter two are little modified (by the order of $(a/r)^3$, where a and r means the cut-off radius and the relative distance) by the prssence of another nucleon in its neighbour. The interaction V of nucleon with unbound mesons can be written as

$$V=S_i e^{i\boldsymbol{q}x},$$

where $\boldsymbol{q}$ means the meson momentum and $\boldsymbol{S}$ denotes the operator concerning spin and isotopic spin variables. An essential point in our discussion is that S has the following selection rule:

$$\Delta j=\pm 1,$$

where j denotes the spin of the nucleon. This means that an ordinary nucleon ($j=1/2$) must necessarily be excited to an isobar ($j=3/2$) when it absorbs a meson. This has the consequence that the possible lowest order process in the π-deuteron absorption is the second order one, being a transition of one of the constituent nucleons to its isobar state by absorbing the meson, followed by the scattering by nuclear potential to ordinary two proton state. As we shall see, this second order process provides the correct angular and energy dependence of the cross section.

We shall denote the total angular momentum, orbital angnlar momentum, spin, and isotopic spin of the two nucleon system by J, L, S and T, respectively. For small meson energies we may replace $\exp(i\boldsymbol{q}\boldsymbol{x})$ in V by unity. In this approximation, $L=0$ in the intermediate state if the initial deuteron is assumed to be in ${}^3S$ state. S and T are either 1 or 2 in the intermediate state and $J=S=1$ or 2. The two proton state can be ${}^1S$, ${}^3P$, ${}^1D$, ..., but from conservation of angular momentum and parity, we obtain the following table of the transition scheme:

	J	L	S	T
initial	1	0	1	0
intermediate	2	0	2	1
final	2	2	0	1

The final state is thus mainly ${}^1D$, if the deuteron is ${}^3S$. This yields, if appropriately summed and averaged over spin state, the $3\cos^2\theta+1$ angular distribution which is in reasonable agreement with observation. Although Durbin et al.[1] obtained the $5\cos^2\theta+1$ instead, the small differences in the coefficient can easily be explained, if the interference of ${}^1D$ with ${}^1S$, which is expected to exist in the final state, is taken into account.

For the evaluation of the cross section, we need an explicit form of the nuclear potential $U(r)$, but the observed increase of cross section can be accounted for in this case, partly because of the energy denominator $1/(E_0-E_{inc})$ ($E_0\approx 280$ Mev means the

isobar energy), and partly because our process is a second order one, which does not require the high momentum Fourier amplitude of the deuteron to go to final state. Since the $U(r)$ derived from strong coupling meson theory[5] suffers from the $1/r^5$ difficulty we have here calculated for the case of less singular potentials, namely

$$U(r)=c\left(\frac{(\boldsymbol{er})(\boldsymbol{er})}{r^2}-\frac{1}{3}(\boldsymbol{ee})\right)\frac{e^{-\mu r}}{r^n}$$

$$+\text{central forces.}\quad (n=1,2)$$

With the simple nuclear wave functions, the second order perturbation calculation is straightforward. The results are drawn in Fig. 1. The coupling constants are adapted by the π-p scattering experiments.

Thus we see that isobar hypothesis furnishes a reasonable understanding for the meso-disintegration of the deuteron. Detailed account will be published later.

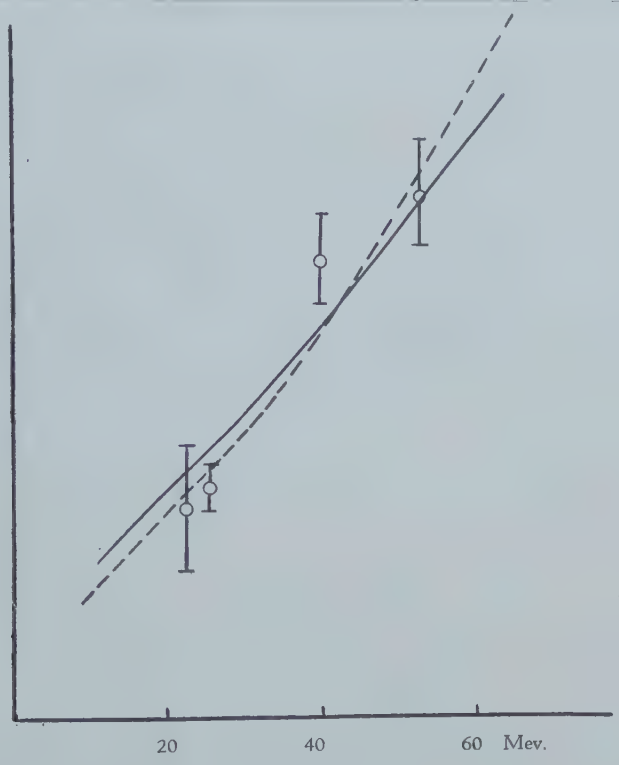

Fig. 1. Total cross section as a function of incident meson energy. Full line for $n=1$, dashed line for $n=2$.

1) R. Durbin, H. Loar and J. Steinberger, Phys. Rev. **84** (1951), 581.
2) W. B. Cheston, Phys. Rev. **83** (1951), 1118.
3) G. F. Chew, M. L. Goldberger, J. Steinberger and C. N. Yang, Phys. Rev. **84** (1951), 581.
4) See in this connection, H. A. Bethe and N. Austern, Phys. Rev. **86** (1952), 121.
5) W. Pauli and S. Kusaka, Phys. Rev. **64** (1943), 400.

Errata

On a Relativistic Integral Equation for Bound States

Chushiro HAYASHI and Yasuo MUNAKATA

(Prog. Theor. Phys. 7 (1952), 481)

p. 490, 18 line, *for* $g_2=2m_2\ell_2$ *read* $g_2=-2m_2\ell_2$.

p. 495, last line, *for* $\{(a_2P_\mu-i\partial/\partial x_\mu{}^2-m_2{}^2\}$ *read* $\{(a_2P_\mu-i\partial/\partial x_\mu)^2-m_2{}^2\}$.

p. 498, last line, *for* (ω_1-m_2) *read* (ω_2-m_2).

p. 500, last line, *for* $-\dfrac{2iWmM}{P}$ *read* $-\dfrac{2iWmM}{P^2}$.

p. 502, 16 line, *for* $\int\int dt'\ r'$ *read* $\int\int dt'\ dr'\ r'$.

18 line, *for* $\int\int dt'\ r'$ *read* $\int\int dt'\ dr'\ r'$.

p. 503, 8 line, *for* $-\dfrac{iMW}{P^2x}$ *read* $-\dfrac{iM}{Px}$.

p. 509, 15 line, *for* $/2j+1,$ *read* $/(2j+1),$.

18 line, *for* $-\pi_2$ (III)′ *read* $-\int\pi_2$(III)′.

18 line, *for* $/2j+1,$ *read* $/(2j+1),$.

p. 510, 12 line, *for* $=\dfrac{1}{2p(W^2+p^2)}$ *read* $=\dfrac{1}{2P(W^2+p^2)}$.

p. 511, Eq. (B. 5), *for* $W^{l+1/2}K_{l+1/2\,(WR)}$ *read* $W^{j+1/2}K^{j+1/2}K_{j+1/2}(WR)$.

Errata

On the Well-ordred S-matrix

Shoichi HORI (Prog. Theor. Phys. 7(1952), 578)

p. 579, line 14, *for* Hamilian *read* Hamiltonian

p. 581, line 12, *for* resyectively *read* respectively

p. 582, 10 lines from bottom, *for* p. 804 *read* p. 581

p. 583, 7 lines from botto n, *for*···$S[a,b,\sigma]$ and between··· *read*···between $S[a,b,\sigma]$ and···

p. 584, 5 lines from bottom, *the number of the Eq. is* (29).

footnote, *for* Eq. (26) *read* Eq. (29).

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On the Formulation of Quantum Mechanics associated with Classical Pictures*

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(Received May 25, 1952)

By re-expressing the generalized Schrödinger equation in its coordinate representation in terms of amplitude and phase of the state vector, a quantum-mechanical change of a system can be made to correspond to an ensemble of classical motions of the system to which is added some internal potential. This ensemble may be taken as the statistical. This enables an alternative formulation of quantum mechanics with which is associated that classical picture. Such a formulation leads, however, if developed straightforwardly according to the picture, to a theoretical scheme quite different from that of ordinary quantum mechanics concerning the problems other than the equation of motion. Furthermore, this formulation is not applicable to Fermions when spin, or exclusion principle is taken into account. Bohm's recent renewed form of the statistical interpretation of quantum mechanics referring to this formulation is criticized in several points. On this formulation we can construct a singular ensemble which is shown to correspond to the tranformation kernel of the wave function to infinitesimally later instant, and thus a connection between this formulation and that of Feynman's is taken out. Hydrodynamical picture formally equivalent to the statistical picture in one-body problems is also considered, and from such analogy certain formal generalization of Schrödinger equation is suggested.

§ 1. Introduction and summary

As is well known we have various different approaches to quantum mechanics, especially the matrix mechanics of Heisenberg, the wave mechanics of Schrödinger, and the space-time approach of Feynman.[1] The purpose of this paper is to explain and to examine another possible approach to quantum mechanics which has the feature of being associated with certain *classical pictures***, and also in this connection to criticize Bohm's recent work[2].

This formulation describes a quantum-mechanical motion of a system by an ensemble of its classical motions, which are referred to single Hamilton-Jacobi function, and which are modified by certain extra potential determined by the density distribution of the ensemble.

This formulation corresponds to the generalization of what was early suggested by de Broglie[3] from the transformed expression of the usual Schrödinger wave equation in terms of amplitude and phase of the wave function.

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* Preliminary report was published in 'Kisokagaku' No. 29 (1952), 30, under the title "The Statistical Picture, the Hydrodynamical Picture and Quantum Mechanics."

** Also the wave formulation of Schrödinger may be pictured as the classical matter field, and when one proceeds on such picture, difficulties in interpretation are produced in like manner as in our case.

Unfortunately this formulation leads to the following inconvenient circumstances. First, it is of such character that the *interpretation* on the basis of the classical picture indicated in the formulation itself contains certain difficulties. We may naturally regard the ensemble stated above as a statistical one, yet such statistical interpretation in terms of extra force field involves conceptual difficulties concerning the probability concept itself, or the discrimination of pure state and Gemisch.

Secondly, this formulation, further developed properly and straightforwardly according to such picture, implies a theoretical scheme considerably different from that of ordinary quantum mechanics as to the problems *other than the equation of motion*. For instance, the probability distributions of various physical quantities are interrelated in different manner; and further, in order to copy the regularity conditions on the wave function, the picture must be subject to some *ad hoc* postulates analogous to the quantum condition in old quantum theory.

Nevertheless, Bohm[2] has recently, on the basis of such picture, attempted a renewed statistical interpretation for quantum mechanics. Roughly speaking, his method to avoid these difficulties is to combine and to compromise this formulation with the usual formulation and also this (statistical) interpretation with the usual interpretation.

To avoid the first difficulties, he imparted to the *wave function* twofold meanings of objectively real *field* and of probability (amplitude), but this interpretation seems to *transfer* the difficulties into the nature of this field.

To avoid the second difficulties, Bohm, though standing upon this picture, regarded the variables of classical orbital motions constituting this picture as *hidden*, while he combined a theory of measurement (which defines the procedure to reproduce observational facts), essentially identical with that of the ordinary interpretation of quantum mechanics. He thus utilized a twofold system of measured values and hidden values for physical quantities, in like manner as he gave the wave function twofold meanings. In this way he was able to manage the statistical interpretation, though in somewhat unnatural manner, so as to lead to the same physical results as in the ordinary interpretation.

Such consequences, inversely speaking, mean that this interpretation as it is brings to quantum mechanics no essentially new functions. His attempts to lead the theory so as to restore some classical picture seem to us in contrary to the probable lines of developments of theory. The idea of hidden variables may be rather interesting in some sense, nevertheless they might not necessarily be representatives of classical concepts such as taken up by Bohm.

In fact, starting from the Einstein's view for the interpretation of quantum mechanics (with sufficient flexibility), he purposely introduced the hidden variables. His general methodological viewpoint set forth in his paper seems rational and interesting. His intent, however, seems not to have been fully incorporated in the procedure taken by him. He has inquired into the possibility to bring back a "precisely defined conceptual model renounced in the usual interpretation of quantum mechanics." Here he has remarked that the 'model' need not be restricted to pictures, and yet what he actually introduced was a picture of classical character. He has intended to provide "a broader *conceptual* framework than

usual interpretation," but the method actually taken by him would, on the other hand, *formally* restrict the further developments of quantum mechanics, because his method implies to base the interpretation of quantum mechanics on the ensemble formulation, whose applicability is, however, rather limited, depending on the formal possibility to transform quantum-mechanical equation of motion into some classical equation of motion.

This formulation is essentially based on the procedure to transform the equation of motion for state vector in its 'coordinate representation' into the form expressing an ensemble of corresponding classical motions. This means, in the first place, that the picture is produced by *fixing* quantum-mechanical change of state in its particular representation in terms of a classical picture not reflecting the invariance property under unitary transformation of quantum mechanics. For this reason the picture has led, as already mentioned, to a theoretical scheme considerably different from that of the ordinary quantum mechanics.

Secondly, the above-mentioned nature of the procedure implies that the range of applicability of the formulation is limited in some measure, for in order the procedure to be feasible there must exist the 'coordinate representation' which makes the system's Hamiltonian expressible as a *differential operator*. Accordingly, e.g., the freedom of spin of electron as particle cannot conveniently be reproduced in this picture, since spin has no conjugate coordinates. Electron as quantum field cannot also be represented in this picture, because in conformity with the exclusion principle there exist no coordinates satisfying *ordinary* commutation relation. The failures are basicaly due to the lack of classical counterparts for them in contrast to the case of electromagnetic field, to which such a picture is applicable. In general this formulation is applicable to Bosons but not to Fermions.

Thus it follows that the coherent application of Bohm's new statistical interpretation for quantum mechanics fails, together with the ensemble formulation, for Fermions, when one takes into account spin, or exclusion principle, more generally that the advanced stage of quantum mechanics may not perfectly be traced in the viewpoint which attempts to hold such pictures as something *essential*.

Conclusively, we can surely regard our formulation of quantum mechanics as a possible one in its limited range of applicability; but we should not take the picture associated with this formulation (i.e., classically defined motion and extra potential) as literally *real*, nor take it as so essential; instead, we should rather consider it as a *medium* to derive, through this formulation, the more essential quantum-mechanical change of state, in a rather similar sense to the path picture in Feynman's formulation. In general one should carefully distinguish the *formulation* and the *interpretation* thereof. Thus in spite of the difficulties in its interpretation, one must be able to treat various problems (equation of motion and stationary state problems) on this fotmulation with no hesitation in utilizing the picture.

For example, on this formulation we can construct the singular ensemble of purely classical trajectories flowing out from a fixed space-time point with any velocity which is shown in a direct manner to correspond to the transformation kernel of the wave function to infinitesimally later instant. This means the Huygens' principle, and thereby a connection between this formulation and the Feynman's (of non-relativistic quantum

mechanics) is taken out.

This formulation is of course also useful in clarifying certain aspect of the correspondence-theoretical relations between classical theory and quantum mechanics[4].

This formulation may also be understood in a hydrodynamical picture for one-particle problems. We can thus describe a quantum-mechanical motion of a particle with an irrotational flow of compressible perfect fluid for case of no magnetic field, and with a rotational flow of certain type when magnetic field present. This picture should again be taken as one in the stage prior to quantum-mechanical concepts. We may however suggest by the help of analogy on these pictures certain formal generalization of Schrödinger equation.

In this connection we also briefly consider the application of formally identical substitution in terms of amplitude and phase to the wave function regarded not as the state vector but as the complex field variable. Quantization of Schrödinger field in this transform according to Bose statistics may suggest its connection to the He II problem. On the other hand we can picture in some degree the electronic spin by a two-fluid model which is much analogous to the two-fluid theory for He II.

§ 2. The picture of an ensemble of trajectories

Schrödinger's wave equation in cartesian coordinates for one spinless particle with Hamiltonian $H(x, p)$:

$$\left\{\frac{\hbar}{i}\frac{\partial}{\partial t}+H\left(x, \frac{\hbar}{i}\nabla\right)\right\}\psi=0, \tag{2·1}$$

can be re-expressed in terms of two real functions R and S meaning amplitude and phase of the wave function ψ respectively, defined by

$$\psi=Re^{(i/\hbar)S}, \tag{2·2}$$

in the form

$$\left\{\left(\frac{\hbar}{i}\frac{\partial}{\partial t}+\dot{S}\right)+H\left(x, \frac{\hbar}{i}\nabla+\nabla S\right)\right\}R=0. \tag{2·3}$$

Taking real and imaginary parts of this equation, we obtain simultaneous equations:

$$\dot{S}-\frac{\hbar^2}{2m}\frac{\Delta R}{R}+H(x, \nabla S)=0, \tag{2·4}$$

$$\dot{P}+\operatorname{div}\left(P\left[\nabla_p H\right]_{p=\nabla S}\right)=0, \tag{2·5}$$

where $P\equiv R^2$ is the probability density.

Now we can reinterpret ('umdeuten') this non-linearized and unsymmetrized form of equation as follows: In the classical limit $\hbar\to 0$, Eq. (2·4) exactly agrees with the classical Hamilton-Jacobi equation of the system; moreover, even if $\hbar\neq 0$, its difference from the latter is merely the fact that it involves an extra term

$$V'(\boldsymbol{x}) = -\frac{\hbar^2}{2m}\frac{\Delta R}{R} = -\frac{\hbar^2}{4m}\left\{\frac{\Delta P}{P} - \frac{1}{2}\frac{(\nabla P)^2}{P^2}\right\} = V'[P(\boldsymbol{x})]\,. \qquad (2\cdot6)$$

This term, which originates from the kinetic energy term $\boldsymbol{p}^2/(2m)$ of the Hamiltonian in $(2\cdot1)$, can be transferred to the potential energy part $V(\boldsymbol{x})$ of $H(\boldsymbol{x}, \nabla S)$ in $(2\cdot4)$; that is, we regard the particle as subject to this '*quantum-theoretical potential*' $V'(\boldsymbol{x})$, as well as the external potential $V(\boldsymbol{x})$. Then Eq. $(2\cdot4)$ is regarded as the classical Hamilton-Jacobi equation under these forces, and

$$[\nabla_p H]_{p=\nabla S} = \boldsymbol{v}(\boldsymbol{x},\ t) \qquad (2\cdot7)$$

is the velocity which a particle shall take if it reaches the point $\boldsymbol{x}$ at time t, moving along one of trajectories derivable from this Hamilton-Jacobi function S. Further, Eq. $(2\cdot5)$, which may now be written as

$$\dot{P} + \operatorname{div}(P\boldsymbol{v}) = 0, \qquad (2\cdot8)$$

means the equation of continuity, regarding P as the density of these moving particles.

Thus we have obtained certain formal *equivalence* between the picture of wave and that of an ensemble of trajectories; more precisely, the Schrödinger's wave motion exactly corresponds to an ensemble of classical orbital motions referred to single Hamilton-Jacobi function under the action of certain extra potential determined by the density distribution of the ensemble. Inversely speaking, if we transfer ourselves from the initial picture of single classical trajectory to that of an ensemble of trajectories derivable from one Hamilton-Jacobi function, only introducing some '*substantial element*', viz., a sort of internal force, but retaining general classical concepts, then we can immediately reach an equivalent of quantum-mechanical change of state. Such circumstances mean another possible approach to quantum mechanics, and suggest the possibility of an alternative formulation of the latter, associated with such classical picture.

The above correspondence, however, does not immediately mean that the formulation based on the picture of an ensemble of trajectories should be able to reproduce the implication of quantum mechanics perfectly; this point will be investigated in some detail in § 5 and the following.

It is evident, however, from the way of its derivation that such formulation is intimately connected with the Schrödinger equation, which is a particular representation of quantum-mechanical equation of motion, expressed in '*Schrödinger representation*' which makes the particle coordinate $\boldsymbol{x}$ diagonal*. We shall explain why it must be so in § 11, but such a situation implies that this formulation does not reflect the characteristic feature of quantum mechanics, the invariance under unitary transformation.

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* It is to be noted that the Schrödinger equation, though in usual is understood further in '*Schrödinger picture*' (i.e., the frame where dynamical quantities are fixed and state vectors change), also is understandable in '*Heisenberg picture.*' Here the state vector ψ is fixed and the particle position $\boldsymbol{x}$ (or any dynamical quantity) as a q number moves, accompanied by the motions of the eigenvectors for this quantity (denoted as $\psi_{\boldsymbol{x}'(t)}$), causing the change of the representative of ψ in this moving frame of $\psi_{\boldsymbol{x}'(t)}$'s. This is what the Schrödinger equation describes. Thus our formulation is not necessarily connected only with the '*Schrödinger picture.*'

Also it is to be noted that for the same reason our method enables us to reveal the correspondence between classical theory and quantum mechanics only in its one specialized aspect.

In the picture indicated in this new formulation, influences of quantum mechanics are visualized as, and concentrated into, the '*blurring*' of the classical trajectory and the appearance of the 'quantum-theoretical potential' which is of such peculiar type as often diverging in the region where $R \to 0$; thus diffusions of wave packets, interference effects, tunnel effects, etc. may be interpreted in terms of this force.

When particular distributions satisfying $\nabla(\Delta R/R)=0$ are allowable, the extra force vanishes and the picture of an ensemble of *purely* classical trajectories gets valid; such solutions will be treated in some detail in § 14.

If there occur no vector potential, and so $H=\boldsymbol{p}^2/(2m)+V(\boldsymbol{x})$, Eqs. (2·7), (2·4), and (2·5) become respectively

$$\begin{cases} \nabla S = m\boldsymbol{v}(\boldsymbol{x},t) = \boldsymbol{p}(\boldsymbol{x},t), & (2\cdot 9) \\ \dot{S} + \dfrac{1}{2m}(\nabla S)^2 + V - \dfrac{\hbar^2}{2m}\dfrac{\Delta R}{R} = 0, & (2\cdot 10) \\ \dot{P} + \operatorname{div}(P\cdot \nabla S/m) = 0. & (2\cdot 11) \end{cases}$$

Our formulation can readily be extended in similar manner to the case of many-particle problems,* by the substitution for probability amplitude (say, for case of two particles)

$$\psi(\boldsymbol{x}_1, \boldsymbol{x}_2) = R(\boldsymbol{x}_1, \boldsymbol{x}_2)\, e^{(i/\hbar)S(\boldsymbol{x}_1, \boldsymbol{x}_2)}, \qquad (2\cdot 12)$$

and the quantum-mechanical change of state of a many-particle system can be pictured as an ensemble of numerous classical motions of this system under the action of certain extra internal forces determined by the density distribution in configuration space of this system.

§ 3. Hydrodynamical picture

We notice at once the above-mentioned picture, for the case of one-particle system, has close analogy with an irrotational flow of a compressible perfect fluid.

The Euler's equation of fluidal motion for the velocity field $\boldsymbol{v}$ is

$$m\left(\frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{v}\nabla)\,\boldsymbol{v}\right) = -\nabla\left(V + \int P^{-1} dp_r\right), \qquad (3\cdot 1)$$

where V/m is the potential of external force per unit mass, P is the density of the fluid (divided by m) considered as a function of pressure p_r. We have besides the equation of continuity:

$$\dot{P} + \operatorname{div}(P\boldsymbol{v}) = 0. \qquad (3\cdot 2)$$

---

* In connection to this case, further see (7·6), § 11(a), and appendix C.

Suppose we substitute the form $V'[P(\rho)]=-(\hbar^2/2m)\Delta R/R$, $(R\equiv P^{1/2})$, for the pressure potential $V_p(P(\rho))=\int P^{-1}dp$, then Euler's equation becomes

$$m\frac{d\boldsymbol{v}}{dt}=m\left(\frac{\partial \boldsymbol{v}}{\partial t}+(\boldsymbol{v}\nabla)\boldsymbol{v}\right)=-\nabla\left(V-\frac{\hbar^2}{2m}\frac{\Delta R}{R}\right). \tag{3·3}$$

The flows under these potential forces persist to be irrotational if initially so, therefore we can restrict our considerations on such flows. Then the volocity field has potential, which we denote as S/m, i.e.

$$\boldsymbol{v}=\nabla S/m, \tag{3·4}$$

and Eq. (3·3), once integrated, reduces to*

$$\dot{S}+\frac{1}{2m}(\nabla S)^2+V-\frac{\hbar^2}{2m}\frac{\Delta R}{R}=0. \tag{3·5}$$

Now Eqs. (3·2), (3·4), and (3·5) are just identical with Eqs. (2·11), (2·9), and (2·10), respectively. This means that the Schrödinger's wave can also be represented by the picture of an irrotational flow of compressible perfect fluid with particular 'pressure' potential.** This potential, being of peculiar type quite different from ordinary ones, brings about unusual forms of flow such as interference, tunnel effect, etc.

The hydrodynamical picture has to be somewhat extended, when the particle is acted on by the electromagnetic field expressed not only with scalar potential ϕ but also with vector potential $\boldsymbol{A}$. We have then the Hamiltonian $H=(1/2m)(\boldsymbol{p}-e\boldsymbol{A}/c)^2+e\phi$ (neglecting spin), and the relation (2·7) takes the form

$$m\boldsymbol{v}=\nabla S-\frac{e}{c}\boldsymbol{A}. \tag{3·6}$$

From this we obtain

$$\operatorname{curl}\boldsymbol{v}=\boldsymbol{\omega}\equiv-e\boldsymbol{H}/mc. \tag{3·7}$$

This relation means that the velocity field is now rotational, and has roticity of Larmor's angular velocity (multiplied by 2) wherever there is magnetic field $\boldsymbol{H}$ present.

Eq. (2·4) is written, for this case, as

$$\dot{S}+\frac{1}{2m}\left(\nabla S-\frac{e}{c}\boldsymbol{A}\right)^2+e\phi-\frac{\hbar^2}{2m}\frac{\Delta R}{R}=0. \tag{3·8}$$

Taking the gradient, we obtain

$$m\frac{d\boldsymbol{v}}{dt}=m\left(\frac{\partial \boldsymbol{v}}{\partial t}+(\boldsymbol{v}\nabla)\boldsymbol{v}\right)=e\left(\boldsymbol{E}+\left[\frac{\boldsymbol{v}}{c}\times\boldsymbol{H}\right]\right)+\nabla\left(\frac{\hbar^2}{2m}\frac{\Delta R}{R}\right). \tag{3·9}$$

This means the Euler's equation under the action of Lorentz force as well as of 'quantum-theoretical force.'

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* From (3·4) alone the velocity potential S is indefinite by an arbitrary function of time, which may suitably be chosen to eliminate the integration constant (allowed to be still a function of time only) which might appear in the right side of (3·5).

** It would be more appropriate to employ the *stress tensor* in place of the pressure potential for the hydrodynamical picture (see appendix A).

§ 4. Some difficulties in the interpretation of the pictures

The hydrodynamical analogy mentioned in the last section, though sometimes useful for the analysis of the Schrödinger equation and rather appropriate to make one visualize the presence of internal force, does not necessarily prove the *reality* of the hydrodynamical picture. In fact such a sort of interpretation as to consider real and continuous distribution of matter would lead to the difficulties similar to those Schrödinger himself early encountered.

On the other hand the statistical interpretation which regards the ensemble stated in § 2 as a statistical one, may also suffer from another difficulties. As is well demonstrated, for example, by interference experiments, the statistical ensemble to be considered in quantum phenomena must be such one referring to a series of *identical experiments* under *equivalent initial conditions* repeated independently from one another. Thus the occurring of internal potential $V'[P(x)]$ has to mean that the force acting on a particle in one experiment be determined by the distribution of the statistical ensemble including that experiment as a member. Such a consequence must hardly be admitted.

To avoid this, Bohm has conceived of a renewed statistical interpretation that in each independent experiment under *equivalent conditions* there occurs always the same potential field which determines the force acting on each particle, and further that on the other hand the probability density of the ensemble be constructed by some reasons so as to get equal to the quantity $P(x)$ which is connected with the potential by a definite relation (2·6). Thus in this view $V'(x)$ is no longer an internal force, but rather a sort of another external force.

Such revision, however, seems to transfer difficulties elsewhere. Generally in statistical interpretations we consider that there exists a classically defined and causally determined motion of particle*, but that as we cannot at least in ordinary cases prepare the motion with perfect precision, we deal with an ensemble of such motions, differing from one another in their initial conditions, (though we above called these mutually differing conditions *equivalent*.) Now by Bohm's idea spatially the same force field must occur irrespective of such variety of initial conditions. This seems unjustifiable.

Bohm has, in fact, regarded $P(x)$ itself as the variable of a real field which determines the force acting on particles by the relation (2·6). Then this field, in spite of its nature of being essentially associated with the particle, determines itself independent of the location of the particle as well as of initial conditions in each experiment, receiving nothing the reaction from the particle. Thus it is conserved and may be normalized, its absolute value of intensity having no significance. These are all its peculiar properties quite different from common fields such as the electromagnetic. Further it must rapidly contract at a measurement, and moreover in many-body problems this quantity $P(x)$ becomes one in configuration space, and so of non-local type as far as we continue to consider it some field.**

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* The statistical interpretation early advocated by Born is considered to be of different type, being rather inherently indeterministic.

** The field itself (for one-particle case) cannot be subject to quantization in this viewpoint, since this leads to violation of the picture (in connection to this point, see § 12).

Bohm has further regarded the quantity ψ itself as mathematical representation of an objectively real field which changes according to the Schrödinger equation, and which on the other hand not only determines the potential field acting on particle in each experiment but also restricts the particle velocity by the relations (2·2), (2·6), and (2·7). Such a compromise of formulations is necessitated, because by the formulation based on S and P one cannot reasonably interpret the *regularity conditions* on ψ. (See § 7).

§ 5. Mean values and 'uncertainty relation'

For the moment we shall take these difficulties in the interpretation out of account, and see in subsequent several sections how the formulation, developed properly and straightforwardly according to such essentially classical picture, may lead to any different consequences from those derived by the quantum-mechanical concept of state, with respect to the problems other than the equation of motion.

First we taken up mean values* of dynamical quantities. As we consider an ensemble defined by S and P, in which particles each with simultaneously determined position $\boldsymbol{x}$ and momentum $\boldsymbol{p}=\nabla S$, are distributed in density $P(\boldsymbol{x})$, the mean value of some dynamical quantity $F(\boldsymbol{x}, \boldsymbol{p})$ over this ensemble at some instant** is to be determined by

$$\langle F\rangle=\int F(\boldsymbol{x}, \nabla S)\,P(\boldsymbol{x})\,d\boldsymbol{x}\,. \tag{5·1}$$

On the other hand the quantum-mechanical mean value (or more precisely the expectation value) of the same quantity referring to the corresponding quantum-mechanical state is given by

$$\langle F\rangle_{\mathrm{qu}}=\int RF(\boldsymbol{x}, \hbar/i\cdot\nabla+\nabla S)\,R\,d\boldsymbol{x}\,. \tag{5·2}$$

Both expressions (5·1) and (5·2) are identical with each other, not only when F is a function of $\boldsymbol{x}$ alone, but also when F is linear in $\boldsymbol{p}$, because of vanishing of the imaginary part of (5·2) due to Hermiticity of F. Thus

$$\langle \boldsymbol{p}\rangle=\int \nabla S\cdot P\,d\boldsymbol{x}=\langle \boldsymbol{p}\rangle_{\mathrm{qu}}\,, \tag{5·3}$$

$$\langle \boldsymbol{l}\rangle=\int[\boldsymbol{x}\times\nabla S]\,P\,d\boldsymbol{x}=\langle \boldsymbol{l}\rangle_{\mathrm{qu}}\,, \tag{5·4}$$

where $\boldsymbol{l}$ is angular momentum of particle.

However for quantities of above 2nd power in $\boldsymbol{p}$, both mean values disagree; for instance $\langle \boldsymbol{p}^2\rangle=\int(\nabla S)^2 P\,d\boldsymbol{x}$, while

$$\langle \boldsymbol{p}^2\rangle_{\mathrm{qu}}=\mathrm{Re}\int R(\hbar/i\cdot\nabla+\nabla S)^2 R\,d\boldsymbol{x}=-\hbar^2\int R\nabla^2 R\,d\boldsymbol{x}+\langle \boldsymbol{p}^2\rangle. \tag{5·5}$$

---

* What we call hereafter *mean values* in the language of the statistical picture, may be translated as *total values* (e.g. 'total momentum' in place of 'mean momentum') in the language of the hydrodynamical picture.

** We may call an ensemble at a given instant 'cloud', about which following problems (mean values, non-dispersiveness etc.) are first investigated.

Since, however, we have regarded the term $V'=-(\hbar^2/2m)\Delta R/R$ as potential, the total energy $E(\boldsymbol{x})$ which particle takes at some point $\boldsymbol{x}$, is exceptionally not equal to $H(\boldsymbol{x}, \nabla S)$, but

$$E(\boldsymbol{x})=H(\boldsymbol{x}, \nabla S)-\frac{\hbar^2}{2m}\frac{\Delta R}{R}=-\dot{S}. \tag{5·6}$$

Its mean value, $\langle E\rangle=\int E(\boldsymbol{x})P d\boldsymbol{x}$, is just equal to the quantum-mechanical mean value,

$$\langle E\rangle_{\mathrm{qu}}=\left\langle\frac{\boldsymbol{p}^2}{2m}+V\right\rangle_{\mathrm{qu}}=\left\langle\frac{\boldsymbol{p}^2}{2m}\right\rangle-\frac{\hbar^2}{2m}\int R\,\Delta R\,d\boldsymbol{x}+\langle V\rangle. \tag{5·7}$$

The composition, however, differs in both viewpoints, a part of kinetic energy in $\langle E\rangle_{\mathrm{qu}}$ being transferred to potential energy in our picture as 'self-potential':

$$\langle V'\rangle=-\frac{\hbar^2}{2m}\int R\,\Delta R\,d\boldsymbol{x}=\frac{\hbar^2}{2m}\int\frac{(\nabla P)^2}{P}d\boldsymbol{x}. \tag{5·8}$$

In practice the kinetic energy alone separated from within the total energy may not be measurable in atomic systems, but the magnitude of angular momentum $\boldsymbol{l}^2$ may be, whose mean values are also given different by both theories; that is,

$$\langle\boldsymbol{l}^2\rangle_{\mathrm{qu}}=\int R\{-\hbar^2[\boldsymbol{x}\times\nabla]^2\}R\,d\boldsymbol{x}+\langle\boldsymbol{l}^2\rangle. \tag{5·9}$$

One might have attained the agreement of both mean values, by adding another new postulate to the picture that the magnitude of angular momentum $\boldsymbol{l}^2$ has 'quantum-theoretical' extra part

$$\lambda[R(\boldsymbol{x})]=-\hbar^2[\boldsymbol{x}\times\nabla]^2 R/R \tag{5·10}$$

at each point, as produced by the gradient of R in non-radial directions. Such an assumption is, however, not justifiable for angular momentum, because it means the violation of the *kinematical* relation between $\boldsymbol{l}^2$ and l_x, l_y, l_z.

We see, according to our picture, the presence of extra internal potential V' gives rise to the accumulation of self-energy* in the ensemble or so-called cloud, which leads the latter to diffusion and gradually transforms into kinetic energy, which this potential, being internal**, has no effect on the motion of the center of gravity (this means Ehrenfest's theorem).

It is possible further to show that there exists a relation between $\langle V'\rangle$ and the dispersion (mean deviation) of particle position, $\overline{\Delta x}$, such that

$$(2mV')^{1/2}\cdot\overline{\Delta x}\geqq\hbar/2, \tag{5·11}$$

in place of the uncertainty relation in ordinary quantum mechanics; while as for the 'uncertainty product' similar to that of quantum mechanics:

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* V' may be positive or negative and often diverges where $R\to 0$, but $\langle V'\rangle$ is always finite, and positive unless P be perfectly uniform.

** Note that $\langle\nabla(\Delta R/R)\rangle=0$.

$$\overline{\Delta x^2}\cdot\overline{\Delta p^2}=(\overline{\Delta x^2}\cdot\overline{\Delta p^2})_{\mathrm{qu}}-\overline{\Delta x^2}\langle 2mV'\rangle,$$

such a relation does not exist.

§ 6. Probability distributions

As is well known the occurence of the so-called *interference of probabilities* is a characteristic feature in quantum mechanics, that is directly connected with the transformation-theoretical constitution of the latter; whereas in our formulation probability distributions of various dynamical quantities are interrelated quite differently corresponding to the fact that our formulation stands on the coordinate representation preferentially.

Though as to mean values our picture has agreed with quantum mechanics for quantities of below first power in $\hbar$, as regards probability distributions* such agreement fails already for quantities of first power in $\hbar$.

In a cloud defined by S and P in our theory, for instance, particle momentum $\boldsymbol{p}$ has definite relation to particle position $\boldsymbol{x}$, $\boldsymbol{p}=\Gamma S(\boldsymbol{x})$, so that in general the probability functions have more intimate correlations and the fluctuation is of quite different type from that of quantum mechanics. Thus the probability distribution in $\boldsymbol{p}$-space, $P(\boldsymbol{p})$, is connected with $P(\boldsymbol{x})$ by

$$P(\boldsymbol{p})\,dp_x dp_y dp_z=P(\boldsymbol{x})\,dx\,dy\,dz\,, \tag{6·1}$$

or

$$P(\boldsymbol{p})\cdot\frac{\partial(p_x,p_y,p_z)}{\partial(x,y,z)}=P(\boldsymbol{x}). \tag{6·2}$$

This means the transformation relation from xyz to $p_x p_y p_z$ is similar to the one from xyz to (e.g.) polar coordicates $r\theta\phi$. The Jacobian in (6·2) is

$$\frac{\partial(p_x p_y p_z)}{\partial(x\,y\,z)}=\det\left|\frac{\partial^2 S}{\partial x_i\partial x_j}\right|. \tag{6·3}$$

In quantum mechanics, on the other hand, the probability for momentum to take a value $\boldsymbol{p}$ in the corresponding state is determined by

$$P_{\mathrm{qu}}(\boldsymbol{p})=h^{-3}\left|\int Re^{i/\hbar(S-\boldsymbol{p}\boldsymbol{x})}d\boldsymbol{x}\right|^2, \tag{6·4}$$

which is quite different from (6·2), giving the same value only to the expressions $\langle\boldsymbol{p}\rangle=\int\boldsymbol{p}P(\boldsymbol{p})\,d\boldsymbol{p}$, and $\int P(\boldsymbol{p})d\boldsymbol{p}(=1)$.

§ 7. Mixing, quantum condition, and superposition

Schrödinger's wave motion has corresponded in our formulation to an ensemble of trajectories, which is not of the most general type, but is restricted to a special collec-

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* The agreement of both probability distributions for $\hbar$ requires that, in terms of mean values, both $\langle\hbar^n\rangle$ and $\langle\hbar^n\rangle_{qu}$ be equal not only for $n=1$ but for every n.

tion of trajectories (of number of ∞^3) derivable from single Hamilton-Jacobi function. When it seems more advisable to express this point explicitly, we shall call such an ensemble ' elementary.'

An elementary ensemble has a fixed momentum field ∇S, (further it is characteristic that this momentum field posseses its potential), so that it can be represented at an instant by a density distribution $P(\boldsymbol{x})$ along a *curve* $\boldsymbol{p}=\nabla S(\boldsymbol{x})$ in phase space, unlike Gibbs' ensemble in classical statistical mechanics, which is reprensented by a density distribution over some *volume* in phase space, and which yields, e.g., the mean value by

$$\langle F\rangle = \int F(\boldsymbol{x},\boldsymbol{p})\,P(\boldsymbol{x},\boldsymbol{p})\,d\boldsymbol{x}\,d\boldsymbol{p}\,, \qquad (7\cdot1)$$

in place of (5·1). Since quantum-mechanical state occupies a phase volume of h^3 in a rough sense, we may say our elementary ensemble is less dispersive than a quantum-mechanical state.

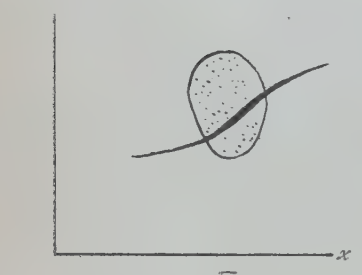

Fig. 1.

Elementary ensemble also differs from Gibbs' ensemble, in that the former involves internal force. For this reason Liouville's theorem is not applicable to it, and thus such as the diffusion of cloud may take place.

Now, from the view-point of our statistical interpretation, more general ensemble, which just like one in classical statistical mechanics occupies a phase *volume*, should equally be considered. Such a general ensemble can be regarded at an instant as a statistical mixture of elementary ensembles. This relation just corresponds to the relation between a *Gemisch* and a *pure state* in quantum mechanics. Further to fit with essential distinctions between pure state and Gemisch, we must assume non-existence of interaction among different elementary ensembles, unlike the presence of internal potential within an elementary ensemble. It implies one of serious difficulties for our statistical interpretation that we must thus assume such discrimination between both types of ensembles which should have equal claim as statistical ensembles. This difficulty may be avoided if we regard the extra potential not as an internal one within the density distribution, but as an external force field which exists, so to speak, previous to the probability distribution of particle, in conformity with Bohm's view.

Quantum-mechanical distinction between pure state and Gemisch may be understandable more simply in the hydrodynamical picture, because here an elementary ensemble is replaced by a real irrotational flow.

In order that elementary cloud or ensemble be such as just to correspond to a wave function ψ, we have to impose a few another conditions on it, corresponding *regularity conditions* for ψ, viz., being finite, continuous, and single-valued. For $\psi=R\exp(iS/\hbar)$ to be single-valued, S need not be necessarily so, but, when azimuth ϕ is taken as one of arguments of S, $\exp(iS/\hbar)$ must be periodic in ϕ with period 2π, accordingly we must have

$$S_{\phi=2\pi}=S_{\phi=0}+mh, \qquad (m:\ \text{integer}). \qquad (7\cdot2)$$

On the other hand if we consider straightforwardly according to our picture, single-valuedness is required also not for S, but for ∇S, differing from (7·2).

With the hydrodynamical language,

$$S_{\phi=2\pi}-S_{\phi=0}=\oint dS=\oint p_s\,ds \tag{7·3}$$

is the circulation of irrotational flow, or the so-called *modulus*. The condition (7·2) is then expressed as

$$\text{modulus}=\oint p_s\,ds=mh\,, \tag{7·4}$$

which is similar to the quantum condition in old quantum theory:

$$\oint p_\phi\,d\phi=mh\,, \tag{7·5}$$

expressed for an orbital motion.

At any rate we are led to a new postulate such as (7·4), which is so to speak the 'quantum condition' for fluidal motion and of *ad hoc* and compromising character for our formulation, just as the quantum condition (7·5) for old quantum theory.

Instead of doing this Bohm has reintroduced the quantity ψ not as a mere mathematical tool but as an objectively real field, imposing on it the same regularity conditions as in wave mechanics. To such idea criticisms stated in § 4 should again be applied.

Just as the condition (7·4), in many-Fermion systems another subsidiary condition is required on its S-function, $S(\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots)$, the condition that S should have the property

$$S(\boldsymbol{x}_2, \boldsymbol{x}_1, \cdots)=S(\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots)+(m+1/2)h, \tag{7·6}$$

for interchange of patticles, corresponding to the exclusion principle.

Besides the procedure of mixing of two elementary ensembles, we can consider also the 'superposition' of the two, which means the procedure to make up an elementary ensemble (S, P) with two such ones (S_1, P_1), and (S_2, P_2), by the rule:

$$c_1 R_1 e^{iS_1/\hbar}+c_2 R_2 e^{iS_2/\hbar}=R e^{iS/\hbar}. \tag{7·7}$$

This equation, or its rewritten form in two real equations, shows the ralation, whereby the two ensembles of trajectories 'interfere' with each other in the region where they overlap.

It is to be noted that in superposition of ensembles constant difference in S does have significance, though from the pictures of trajectory ensemble or of irrotational flow, it is $S=-E(\boldsymbol{x})$ and $\nabla S=\boldsymbol{p}(\boldsymbol{x})$ that have physical significance, S itself having arbitrariness by any additive constant.

§ 8. Non-dispersive clouds

Next we shall consider the cloud in which certain dynamical quantity $F(\boldsymbol{x}, \boldsymbol{p})$ takes single non-dispersive value, F'.

Such a cloud is obviously defined by

$$F(\boldsymbol{x}, \nabla S) = F', \tag{8·1}$$

except for the case when F means energy.* As this equation involves only S but not P, the non-dispersive cloud is characterized by its velocity field. Furthermore Eq. (8·1) is purely classical one, not involving $\hbar$, so the condition to be non-dispersive is not expected to be able to lead to any discrete quantization. In quantum mechanics, on the other hand, the state which makes the quantity $F(\boldsymbol{x}, \boldsymbol{p})$ non-dispersive is its eigenstate, to be determined by

$$F(\boldsymbol{x}, \hbar/i \cdot \nabla + \nabla S) R = F' R . \tag{8·2}$$

For quantities of first power in $\boldsymbol{p}$, Eq. (8·1) agrees with the real part of (8·2), but the latter involves another relation. For example, the eigenstate for momentum is determined by (8·2) as

$$\begin{cases} \nabla S = \boldsymbol{p}' & \therefore \ S = \boldsymbol{p}' \boldsymbol{x} + S'(t), \qquad (8·3) \\ \nabla R = 0 & \therefore \ R = R(t), \qquad (8·4) \end{cases}$$

whereas in our picture non-dispersive cloud for momentum is determined only by (8·3). This is an example to show uncertainty relation to fail. In order, however, that such non-dispersive cloud be maintained for course of time, the ensemble must also satisfy the equations of motion (2·10) and (2·11). Then we get $P = \text{const.}$ and $V = 0$, namely the non-dispersive *ensemble* for momentum is only possible in free space as $S = \boldsymbol{p}' \boldsymbol{x}$, $P = \text{const.}$, just as in quantum mechanics.

Similarly the eigen-state for z-component of angular momentum l_z is defined by

$$\begin{cases} [\boldsymbol{x} \times \nabla S]_z = \dfrac{\partial S}{\partial \phi} = l_z', \qquad (8·5) \\ [\boldsymbol{x} \times \nabla R]_z = \dfrac{\partial R}{\partial \phi} = 0, \qquad (8·6) \end{cases}$$

while in our picture non-dispersive cloud for l_z is expressed only by (8·5), from which we obtain,

$$S = l_z' \phi + S'(r, \theta, t). \tag{8·7}$$

Now if we simply stand upon our picture, the requirement of single-valuedness is to be applied on ∇S, and this is fulfilled by (8·5) itself. So we obtain no discrete quantization from the condition to be non-dispersive. If we, however, here apply the 'quantum condition' (7·4) to (8·7), we obtain discrete eigen-values

$$l_z' = m\hbar, \qquad (m : \text{integer}). \tag{8·8}$$

For quantities quadratic in $\boldsymbol{p}$, Eq. (8·1) no longer even agrees with the real part of (8·2). For example, again for the magnitude of angular momentum $\boldsymbol{l}^2$, Eq. (8·2) takes the form

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* For this case, see next section.

$$[x\times\nabla S]^2+\lambda(x)=\lambda', \tag{8·9}$$

$$\{[x\times\nabla][x\times\nabla S]+[x\times\nabla S][x\times\nabla]\}R=0. \tag{8·10}$$

If we want to interpret the relation (8·9) according to our picture, we might again have to resort to the extra 'quantum-theoretical' part of angular momentum, $\lambda(x)$ [Eq. (5·10)].

In general, if we reexpress an eigenvalue equation in quantum mechanics as two real equations for S and R, the real part equation may be interpreted on our picture, though in some cases by makeshift procedure of extra 'quantum-theoretical' term, but the imaginary part equation expresses another relation not necessitated from our picture. Only for energy, both relations of eigen-value equation may be interpreted on our picture, like the equation of motion itself, because the eigen-state of energy agrees with the stationary state of *motion* (for this see next section). On the other hand, quantum-mechanical mean value is defined, as was stated in § 5, only by the relation corresponding to the real part equation, so that it has been interpreted, though sometimes by means of extra 'quantum-theoretical' term.

§ 9. Stationary ensemble

From our pictures the conditions that an ensemble (or flow) should be stationary are to be defined by

$$P=0, \qquad \frac{\partial}{\partial t}\nabla S=0. \tag{9·1}$$

From the second of above equations, we obtain $S=S'(x)+S''(t)$, so Eqs. (2·11), (2·10), and (5·6) reduce to

$$\operatorname{div}(P\nabla S')=0, \tag{9·2}$$

$$E(x,t)=-\dot{S}''=H(x,\nabla S')-\frac{\hbar^2}{2m}\frac{\Delta R}{R}. \tag{9·3}$$

Eq. (9·3) is fulfilled only when it is equal to a constant, hence it follows that

$$E(x,t)=E, \tag{9·4}$$

$$S=-Et+S'(x), \tag{9·5}$$

$$H(x,\nabla S')-\frac{\hbar^2}{2m}\frac{\Delta R}{R}=\frac{1}{2m}(\nabla S')^2+V-\frac{\hbar^2}{2m}\frac{\Delta R}{R}=E. \tag{9·6}$$

Thus in a stationary ensemble energy takes a non-dispersive value and remains so, just as in a stationary state in quantum mechanics. Inversely, however, a non-dispersive ensemble for energy in our picture is not necessarily a stationary one, as P may still depend on t.

Eqs. (9·2) and (9·6) which determine our stationary ensemble are equivalent to the rewritten from of $H\varphi=E\varphi$ (φ being space eigen-function) by the substition $\varphi=R\exp(iS'/\hbar)$, that is

$$H(x, \hbar/i \cdot \nabla + \nabla S') R = ER\,, \tag{9·7}$$

which is a special case of (8·2). It is also noted that with the language of hydrodynamical picture, Eq. (9·6) expresses the *Bernoulli's theorem* for stationary flow (for the case of irrotational motions).

For a stationary state thus we have equations equivalent to the equation of wave mechanics, and therefore it seems possible to derive just the same energy eigen-values and 'eigen-ensembles' as those of wave mechanics. Really, it is possible only when we take into account the conditions such as (7·4), corresponding to the regularity condition on ψ.

For example we consider the solution of (9·2), and (9·6) such that S' depends on ϕ alone and P depends on r, θ alone. From (9·2) we get

$$S' = \text{const.} \cdot \phi = l_z' \phi\,. \tag{9·8}$$

Here the const., l_z', meaning the non-dispersive value of the component of angular momentum, may take any value from our original picture; hence Eq. (9·6) inserted with (9·8) does not yield energy eigen-values discrete. Only by taking (7·4) and so (8·8) into account we get identical results with those of wave mechanics.

Eq. (9·2) is satisfied by static clouds $\nabla S' = 0$. Eq. (9·6) then reduces to

$$-\frac{\hbar^2}{2m}\frac{\Delta R}{R} + V = E\,,$$

which is identical with the Schrödinger's stationary state equation, taking into account that now $\varphi = R$. In particular the lowest stationary cloud belongs in general to such static one, and can also be determined by the variational theorem:

$$\langle E \rangle = \int \left\{ VP + \frac{\hbar^2}{8m} \frac{(\nabla P)^2}{P} \right\} dx = \min., \quad (\int P dx = 1). \tag{9·9}$$

This implies that the total potential energy as the sum of potential energy due to external force and the self-energy, should take a minimum, or in other words that the application of the classical equilibrium theorem in hydrodynamical picture is effective.*

§ 10. Interpretation regulated with the theory of measurements

We have seen in previous several sections that the picture of the ensemble of trajectories leads to different results from those of quantum mechanics, with respect to such problems as probability distributions or non-dispersive values of dynamical quantities. However, as Bohm[2] has shown, it is possible to regulate our statistical interpretation so as to enable the agreement with ordinary interpretation of quantum mechanics in regard to physical results derivable therefrom.

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* Generally speaking, the motion can be derived by the variational principle: $\delta \int\int \mathfrak{L}\, dx\, dt = 0$, where $\mathfrak{L}$ is given by (12·2) (see § 12).

This is accomplished by regarding the practically observed values of physical quantities as another things from the values which the picture directly yields, and moreover by introducing such a theory of measurement processes to reproduce the measured values as is essentially identical with that in ordinary interpretation. Stating more explicitly, one distinguishes the measured value of a quantity and the value 'really' taken by this quantity before (or in course of, or after) the measurement, and considers that to measure a quantity F does not mean to know the value 'really' taken by this quantity as it is—this is impossible—, but means to insert such an interaction between the system under consideration and a suitable measuring apparatus as to lead to separating the initial ensemble (R, S) into 'eigen-ensembles' $(R_{F'}, S_{F'})$ corresponding to the quantum-mechanical eigenstates $\psi_{F'}$ for this quantity, each of which is combined with each of apparatus, 'wave-packet states' (i.e. ensembles of small dispersion for coordinate), which in turn corresponds to a *reading*. Such a separation may be considered to mean that as the result of measurement, the ensemble turns from its initial form (R, S) into any of eigen-ensembles $(R_{F'}, S_{F'})$ each with definite probability, together with the apparatus indicating each a certain reading corresponding to F'; thus in accordance with this latter fact one states, "The measured value of the quantity F is F'."

In this course of measurement, on the other hand, the probability distribution of values 'really' taken by F turns from its initial form for (R, S) into the form for $(R_{F'}, S_{F'})$, which, in fact, corresponds to a non-dispersive ensemble of F taking F' in case of most of quantities usually measured (position, momentum, energy, etc.), as has been seen in § 8; though here remains a gap, e.g., for magnitude of angular momentum.

One can further interpret transition processes in general in much the same way.

This interpretation is based on the transformed expression of the equation of motion and the probability interpretation both for coordinate representation of state vector (referring not only to the system under observation but also to the composite system which may consist of parts interacting with each other and thus inducing transitions). Since these have been taken essentially identical as in quantum mechanics, it has been possible to construct interpretation such that transition or measurement processes reveal not the general non-dispersive ensembles stated in § 8, but the eigen-ensembles (and eigenvalues) in accordance with ordinary interpretation.

In this interpretation, however, one had to adopt it as a fundamental postulate that measuring some quantity means to insert such an interaction between the system and a suitable apparatus as to separate the initial ensemble into eigen-ensembles (corresponding to the quantum-mechanical eigenstates) for this quantity. This postulate, though in itself in harmony with general properties of measurement, is not so natural as in ordinary quantum mechanics which stands on the state concept based on the superposition principle.

This interpretation of measurement process, though essentially equivalent to that of ordinary interpretation, might be somewhat more intelligible with respect to the statistical character of results of a measurement, since here the definition of state is statistical from the outset.

In passing the distinction between elementary ensembles and their mixture, remarked

in § 7, is now more obvious: The situation in which the particle certainly belongs to one of elementary ensembles can be prepared, but it is impossible further to know which motion in this elementary ensemble actually takes place.

This interpretation, with its twofold system of measured values and hidden values for physical quantities, is capable of retaining the same physical results as in ordinary quantum mechanics on the one hand, and at the same time of having the picture of ensemble of trajectories on the other hand. However, as far as this interpretation lets the theory imply such procedure to reproduce observational facts as is essentially equivalent to that of ordinary quantum mechanics, the interpretation essentially consists in introducing into quantum mechanics the quantities such as simultaneously defined position and momentum of particle as 'hidden variables,' inobservability of which is guaranteed by the theory itself, and which only play the role to make the classical picture possible. Apart from the fact that such a picture itself is not free from difficulties as pointed out in § 4, such hidden variables as it is may be said to be metaphysical superfluities so far as they have no connection with observations in the end*.

Bohm attempted to impart radical significance to introducing hidden variables into quantum mechanics by the help of analogy of classical atomic theory introduced into classical macroscopic theory. Such analogy, however, should be treated more carefully.

The atomic theory has introduced into phenomenological theory *physical entities* provided with *freedoms* of motion described by dynamical variables as well as with *structure constants* (atomic mass, elementary charge, etc.), which may be regarded for the phenomenological theory as hidden variables and '*hidden constants*'; moreover it considered a macroscopic system as an *assembly* of a great number of these entities, and also a macroscopic state as a statistical *ensemble* of microscopic states of this assembly, (here taking Gibbs' viewpoint rather than Boltzmann's).

Introducing hidden variables into quantum mechanics is quite different in its significance from the above case. This method consists in substituting an (elementary) *ensemble* of trajectories each defined by particle position and momentum as c-numbers for a motion described by particle position and momentum as q-numbers referred to some fixed state vector (here using Heisenberg picture). Thus it implies to alter the concept of motion in any freedom of the entity, rather than to introduce another new physical entities provided with freedoms of motion and with structure constants (so there could exist correspondence), apart from the difference, as to the degree in which one considers the wave function something substantial, among the viewpoints such as hydrodynamical interpretation, 'quantum-theoretical' potetial interpretation, ordinary interpretation, etc.

If we interpret the word 'hidden variables' or hidden constants more broadly, Planck's constant may be said as a sort of hidden constant for classical theory. It is no structure constant itself and led to the alteration of logic of classical theory. Likewise Heisenberg's universal length might be some hidden constant for present quantum theory.

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* More precisely, the definite position of particle might be admitted since the probability distribution for positional measurements is directly given by $P(x)$, but simultaneously definite momentum might not since the probability distribution for momentum measurements is not given by $P(p)$ as was explained in § 6.

Quantum mechanics may be regarded itself as an '*essentialistic*' theory,[5] and there seems to be no reason to suspect that there exist something hidden, as far as we confine ourselves within non-relativistic quantum mechanics.[6] If we are to introduce into this theory some new element which alters its *logic*, may it be hidden variables or others, it is expected to be such as to make the phenomenological elements in quantum field theory derivable from within the theory itself as well as to resolve some intrinsic difficulties in the present quantum mechanics when applied to fields.

Now to introduce definite position and momentum of particle as hidden variables brings to quantum mechanics no essentially new functions by itself. Essentially new role of these hidden variables arises only when the Schrödinger equation is modified so as to make the hidden variables no longer hidden. Such a way of modification of Schrödinger equation is somehow suggested from the viewpoint of this new interpretation. Along this line Bohm has in fact tried certain modifications, which seem, however, to the author rather artificial and improbable*. (We shall suggest formally a little more natural generalization of Schrödinger equation in § 13.)

The general idea to introduce some hidden variables into quantum mechanics is rather interesting, but there seems to be no reason for them to be classical quantites such as the definite position and momentum of particle. Besides these quantities another classical concept, (extra) potential of force (which should not be subject to quantization), must also be introduced into this interpretation. To proceed thus as to restore some classical picture may not be regarded as going along any probable lines of developments of the theory.[7] Although such attempts have at least formally been feasible for the case of customary Schrödinger equation which corresponds to a non-relativistic orbital motion of particle, similar procedure will not successfully be formulated for Fermions if spin or exclusion principle are taken into account (see next section).

Conclusively (from what we have seen, especially in § 4 and in this section, and also shall see in the next section), although our formulation of quantum mechanics offers the 'fourth' possible one within its limited range of applicability, we should not take the picture associated with this formulation (i.e. classically defined motion and special extra force) as literally *real*, nor take it as so essential; instead, we should rather consider it as a *medium* to derive the more essential quantum-mechanical change of state through this formulation. The applicability of the formulation has been clarified in § 5～9 with respect to one side of the problem and will be analized in the next section as to the other side.

§ 11. Applicability of the method

Electromagnetic field, spin, relativity and statistics

We shall now investigate, from a standpoint more general than that taken in § 2, in what scope such formulation is applicable, that represents a quantum-mechanical change

* In this trial Bohm adopted it as another guiding postulate that such modifications should only begin to be effective "in the domains associated with dimensions of the order of 10^{-13} cm, where the extrapolation of the present quantum theory seems to break down." It seems, however, unjustifiable to explore the law of motion in such domains on the basis of non-relativistic Schrödinger equation for spinless particle.

of state of some system (with Hamiltonian H) described in a generalized Schrödinger equation for state vector Ψ:

$$\left(\frac{\hbar}{i}\frac{\partial}{\partial t}+H\right)\Psi=0\,, \tag{11·1}$$

by an ensemble of corresponding classical motions.

(a) General procedure

Eq. (11·1) takes the form*:

$$\frac{\hbar}{i}\frac{\partial}{\partial t}(\xi'|)+\int(\xi|H|\xi'')(\xi''|)d\xi''=0\,, \tag{11·2}$$

referred to one of representations which is assumed to make some quantity $\hat{\xi}$ diagonal, adopting here Dirac's notation. We know that the conservation relation for probability holds for $|(\xi'|)|^2$:

$$\frac{d}{dt}\int|(\xi'|)|^2d\xi'=0\,, \tag{11·3}$$

guaranteed by the Hermiticity of H. In order that the state, *through this representation*, should correspond to a statistical ensemble of classical states, we should still adopt the quantity $|(\xi'|)|^2$ as the probability density of this ensemble, because it is the quantity satisfying the condition (11·3). We must, however, now reinterpret it as meaning the probability that the quantity $\hat{\xi}$ 'really' takes the value ξ', so as to be in harmony with classical state concept.

To transform the quantum-mechanical equation of motion (11·2) into the form corresponding to the picture of a statistical ensemble of classiaal motions, we are then to adopt the quantity $|(\xi'|)|^2=P$ or $|(\xi'|)|=R$ as one of state variables. Separating this factor from $(\xi'|)$, we get the residual of absolute value unity, which should be expressed as $\exp(iS/\hbar)$ using another real quantity S (the unit $\hbar$ being taken for convenience). Consequently we are led to the substitution

$$(\xi'|)=R(\xi')e^{iS(\xi')/\hbar}. \tag{11·4}$$

For such a substitution to meet our purpose, however, it must be one referred to such a representation as to make the Hamiltonian a *differential operator*, since in this case the factor $\exp[iS(\xi')/\hbar]$ in (11·4) turns back to itself (multiplied by $(i/\hbar)\partial S/\partial\xi'$) through differentiation involved in the Hamiltonian operator and so drops off from the equation of motion (11·2) which is linear and homogeneous in $(\xi'|)$.

In order that the Hamiltonian, generally taking a form of an integral operator or a matrix, specially be expressible as a differential operator, first, it must be expressible as a function of suitable canonical variables**, q and p, satisfying *ordinary* commutation relation:

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* Integral means summation when ξ takes discrete eigenvalues.

** We further consider q and p as Hermitian operators, taking real eigenvalues, so as conveniently to separate Eq. (11·6) into its real and imaginary parts.

$$pq-qp=\hbar/i\,. \tag{11·5}$$

In this case in the representation which makes q diagonal, p is expressed as $(\hbar/i)\partial/\partial q$, or vice versa.

Now suppose H is expressible as a power series in p but not (necessarily) in q, then it is expressible as a differential operator in q-representation but not (necessarily) in p-representation. In such a case, by taking the substitution (11·4) in q-representation, (11·2) becomes*

$$\left\{\left(\frac{\hbar}{i}\frac{\partial}{\partial t}+\dot{S}\right)+H\left(\cdots q_i,\ \frac{\hbar}{i}\frac{\partial}{\partial q_i}+\frac{\partial S}{\partial q_i}\cdots\right)\right\}R=0. \tag{11·6}$$

This may be separated into two real simultaneous differential equations. The real part equation (for $\dot{S}$) evidently agrees with the classical Hamilton-Jacobi equation except for the term of above 2nd order in $\hbar$, the imaginary part equation (for $\dot{R}$) meaning the equation of conservation of probability.

Further, it is sufficient to restrict H to be *quadratic* in each p_i, allowing of *cross-terms*, (and of course Hermitian), such that,

$$H=\sum_{ij}\frac{1}{2}\left(a_{ij}p_ip_j+p_ip_ja_{ij}\right)+\sum_i\frac{1}{2}\left(b_ip_i+p_ib_i\right)+V, \tag{11·7}$$

where each a_{ij}, b_i, and V may be real functions of q_i's. Then real and imaginary part equations of (11·6) are shown to be

$$\dot{S}+H\left(\cdots q_i,\ \frac{\partial S}{\partial q_i}\cdots\right)+V'\left[R(\cdots q_i\cdots)\right]=0, \tag{11·8}$$

$$\dot{P}+\sum_i\frac{\partial}{\partial q_i}\left[P\left(\frac{\partial H}{\partial p_i}\right)_{p_i=\partial S/\partial q_i}\right]=0, \tag{11·9}$$

respectively. Here

$$V'=-\frac{\hbar^2}{2R}\sum_{ij}\left\{a_{ij}\frac{\partial^2 R}{\partial q_i\partial q_j}+\frac{\partial^2}{\partial q_i\partial q_j}\left(a_{ij}R\right)\right\}. \tag{11·10}$$

Eq. (11·8) is the classical Hamilton-Jacobi equation for the system with Hamiltonian

$$\bar{H}=\sum_{ij}a_{ij}p_ip_j+\sum_i b_ip_i+V+V'=H+V', \tag{11·11}$$

in which V' means the extra potential. For (classical) motions derivable from this Hamilton-Jacobi function,

$$\frac{dq_i}{dt}=\left(\frac{\partial\bar{H}}{\partial p_i}\right)_{p_i=\partial S/\partial q_i}=\left(\frac{\partial H}{\partial p_i}\right)_{p_i=\partial S/\partial q_i},$$

hence (11·9) means the conservation of probability in q_i-space. We could thus infer in these cases the validity of the picture of an ensemble of corresponding classical motions (to which is added the extra potential determined by the density distribution in con-

* Here we specify various freedoms by subscript i, and denote eigenvalues of q_i merely as q_i.

figuration space) for a quantum-mechanical change of state of a system.

The cases treated in § 2 naturally belong to what now considered. The Hamiltonian of a particle or particles without spin has potential $V(\boldsymbol{x})$ or $V(\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots)$, not in general a power series in $\boldsymbol{x}$ or $\boldsymbol{x}_i$. For this reason we had to resort exclusively to the coordinate representation.

Our formulation is thus connected with a particular representation and has not the meaning invariant under unitary transformations.*

(b) Electromagnetic field and other Bose fields

The procedure in (a) is evidently applicable to electromagnetic field, because it may be regarded as an assembly of oscillators. To see this more explicitly, we briefly consider the electromagnetic field in vacuum in its most elementary form : We represent the field with its vector potential $\boldsymbol{A}$, which is expressed in fourier expansion in volume V as

$$\boldsymbol{A}=\sum_{\lambda} q_\lambda \boldsymbol{u}_\lambda(\boldsymbol{x}), \qquad \boldsymbol{u}_\lambda(\boldsymbol{x})=V^{-1/2}\boldsymbol{e}_\lambda \begin{matrix}\cos\\ \sin\end{matrix} \boldsymbol{k}\boldsymbol{x}\,, \tag{11·12}$$

where q_λ's are real, λ specifying in a lump the propagation vector $\boldsymbol{k}$, polarization direction $\boldsymbol{e}_\lambda$, and cos or sin component.

The equations of motion are derived from the Hamiltonian

$$H(\cdots q_\lambda, p_\lambda \cdots)=\sum_{\lambda}\frac{1}{2}(c^2 p_\lambda{}^2+k^2 q_\lambda{}^2), \tag{11·13}$$

which corresponds to an assembly of oscillators each with q_λ, p_λ as canonically conjugate variables satisfying ordinary commutation relations. We then get equations similar to (11·8) and (11·9) with H taken as (11·13), and so the quantum-mechanical change of state of electromagnetic field can be represented by an ensemble of classical motions of the field with extra potential

$$V'=-\frac{\hbar^2 c^2}{2R}\sum_{\lambda}\frac{\partial^2 R}{\partial q_\lambda{}^2},$$

to be determined by the density distribution in the coordinate space of field oscillators.

In this picture $p_\lambda=\partial S/\partial q_\lambda$ as well as q_λ have simultaneously defined values, accordingly the electric and magnetic field strengths, $\boldsymbol{E}$, $\boldsymbol{H}$ at every space-time point also have simultaneously defined values, which mean the 'hidden variables' in this case.

In this picture the mean values of $\boldsymbol{E}$ and of $\boldsymbol{H}$ agree with those in quantum-mechanics, and satisfy Maxwell equations. The mean values of field momentum $\boldsymbol{G}$, and of field energy, too, as far as V' is taken into account as potential energy, also agree with those of quantum mechanics. The stationary state is a static ensemble, where the electric field vanishes and only the static magnetic field survives.

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* The substitution (11·4) in some particular representation is not unitary invariant. This is for the same reason that state vector cannot be split up into its real and imaginary parts.

Since in these problems (also see Eq. (11·38)), the system may be reduced to an assembly of *oscillators* whose Hamiltonian is symmetrical in p and q, our procedure can be carried out in similar manner through the similar substitution for p-representation of state vector :

$$\Psi(\cdots p_\lambda \cdots, t) = R \exp(iS/\hbar).$$

We can handle the problem in a similar way, even if the interaction with several charged particles may occur, as far as we treat the latter in non-relativistic approximation neglecting spin, because the interaction Hamiltonian,

$$H' = -\frac{e}{2mc}(\boldsymbol{pA} + \boldsymbol{Ap}) + \frac{e^2}{2mc^2}\boldsymbol{A}^2$$

is linear in $\boldsymbol{p}$ (particle momentum) with the coefficient which is only a function of q_λ's.

It would be desirable that our formulation might be such as to suggest an idea for some modification of present theory in the treatment of *interaction* where the present theory encounters some difficulties. We cannot however proceed immediately to investigate this point, since, as we shall see our formulation cannot reproduce the present quantum theory for some *free* systems which has proved its sufficient legitimacy and is expected to be essentially retained in future theory.

Our procedure is applicable to *Bose fields* in general, not limited to electromagnetic field. For instance, we take up the complex vector field ('vector meson') with mass and charge. Its Hamiltonian is expressed in fourier expansion as[8]

$$H = \sum_k \left\{ c^2(\boldsymbol{p}_k^* \boldsymbol{p}_k) + \frac{\hbar^2}{m^2}(\boldsymbol{k}\boldsymbol{p}_k^*)(\boldsymbol{k}\boldsymbol{p}_k) + \frac{m^2c^2}{\hbar^2}(\boldsymbol{q}_k^*\boldsymbol{q}_k) + ([\boldsymbol{k}\times\boldsymbol{q}_k^*]\cdot[\boldsymbol{k}\times\boldsymbol{q}_k]) \right\}, \tag{11·14}$$

with p_{kj}, q_{kj} (components of vectors $\boldsymbol{p}_k$, $\boldsymbol{q}_k$) as canonical variables satisfying ordinary commutation relations :

$$[p_{kj}, q_{k'j'}] = [p_{kj}^*, q_{k'j'}^*] = (\hbar/i)\delta_{kk'}\delta_{jj'}.$$

The Hamiltonian is again quadratic in each p_{kj} and q_{kj}, accordingly also quadratic in the real canonical variables obtainable from p_{kj} and q_{kj} by their linear combinations, and so we can then apply the procedure in (a). It will be further possible to separate the freedoms perfectly by decomposing each $\boldsymbol{p}_k$, $\boldsymbol{q}_k$ into longitudinal and transversal components, and to reduce the system to an assembly of oscillators, just as in the case of electromagnetic field ; but our procedure is feasible as well for the form of H including cross-terms such as (11·14).

(c) Eletcronic spin and two-fluid model

The procedure, however, is not applicable to a particle with spin even in non-relativistic approximation ; since the spin of a particle is of essentially quantum-mechanical nature, without its counterpart in classical particle mechanics, so that the freedom of spin in quantum mechanics can hardly be projected upon any collection of classical particle motions.

In other words, as for the freedom of spin, since there exist no coordinate conjugate to spin angular momentum, or none of any other mutually conjugate variables satisfying ordinary commutation relation, we have no 'coordinate representation' of the generalized Schrödinger equation (11·1), which is essential for the procedure as was explained in (a).

In the case of electromagnetic field, both the classical and quantum-mechanical theories were field theories from the beginning, mutually transmutable through the ordinary commutation relation (11·5), so the classical field involved the freedoms corresponding to the 'spin' of photon as polarizations; thus there existed the correspondence between a quantum-mechanical motion and an ensemble of classical motions.

The situation may also be explained as follows: Due to the non-commutability of σ or γ (in case of Dirac equation) matrices, the wave equation for electron has inseparable character for each independent component of wave function (which is now considered as state vector), so that, on inserting

$$\psi_\rho = R_\rho \exp(iS_\rho/\hbar), \tag{11·15}$$

exponential factors do not drop off from the equation. Hence, the separation into real and imaginary parts brings terms including cos or $\sin(S_\rho/\hbar)$. This leads to violation of our procedure.

To illustrate this, we shall consider in non-relativistic approximation the case when only magnetic field H present. By the substitution (11·15), the wave equation, (taking for spin the *particular* representation which makes σ_z diagonal), separates into four simultaneous equations:

$$\dot{S}_1 + \frac{m}{2}\boldsymbol{v}_1^2 - \frac{\hbar^2}{2m}\frac{\Delta R_1}{R_1} + \hbar g H_z + \hbar\frac{\gamma}{P_1} = 0\,, \tag{11·16}$$

$$\dot{S}_2 + \frac{m}{2}\boldsymbol{v}_2^2 - \frac{\hbar^2}{2m}\frac{\Delta R_2}{R_2} - \hbar g H_z + \hbar\frac{\gamma}{P_2} = 0\,, \tag{11·17}$$

$$\dot{P}_1 + \operatorname{div}(P_1\boldsymbol{v}_1) + 2\delta = 0\,, \tag{11·18}$$

$$\dot{P}_2 + \operatorname{div}(P_2\boldsymbol{v}_2) - 2\delta = 0\,. \tag{11·19}$$

Here $g \equiv -e/2mc$, and

$$\boldsymbol{v}_i = (\nabla S_i - c\boldsymbol{A}/c)/m\,, \tag{11·20}$$

$$\gamma = gH_\perp R_1 R_2 \cos[(S_1 - S_2)/\hbar + \alpha]\,, \tag{11·21}$$

$$\delta = gH_\perp R_1 R_2 \sin[(S_1 - S_2)/\hbar + \alpha]\,, \tag{11·22}$$

$$(H_\perp = (H_x^2 + H_y^2)^{1/2},\quad \tan\alpha = H_y/H_x).$$

Further, taking the gradient of (11·16) and (11·17), we obtain

$$m\frac{d\boldsymbol{v}_1}{dt} - e\left[\frac{\boldsymbol{v}_1}{c}\times H\right] - \nabla\left(\frac{\hbar^2}{2m}\frac{\Delta R_1}{R_1}\right) + \hbar g\nabla H_z + \hbar\nabla\left(\frac{\gamma}{P_1}\right) = 0\,, \tag{11·23}$$

$$\hbar\Gamma\left(\frac{\gamma}{P_1}\right)=\hbar g\Gamma\left(H_\perp\cdot R_2/R_1\right)\cdot\cos\left[\left(S_1-S_2\right)/\hbar+\alpha\right]-m(\boldsymbol{v}_1-\boldsymbol{v}_2)\,\delta/P_1=0 \qquad (11\cdot24)$$

and the analogous equation for (11·17).

These equations may be interpreted as follows: We consider, as in the case of liquid He II in the two-fluid theory, two mutually interpenetrating fluids, which have velocity fields $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$ (derivable from velocity potentials S_1 and S_2 by the relation (11·20)) and density distributions P_1 and P_2, respectively. Then Eqs. (11·18) and (11·19) show that the first fluid is changing into the second at the rate of 2δ at each point. This requires the momentum supply of $m(\boldsymbol{v}_2-\boldsymbol{v}_1)\cdot 2\delta$, which is *equally* allotted to both liquids as reaction force $m(\boldsymbol{v}_1-\boldsymbol{v}_2)\delta$ (appearing in (11·24)), just as in the two-fluid theory[9] of He II.

Besides this reaction, each fluid is subject to Lorentz force (see § 3), usual 'quantum-theoretical' force, and 'quantum-theoretical' magnetic force:

$$K_1=-\hbar g\left\{\Gamma H_z+\Gamma\left(H_\perp\cdot R_2/R_1\right)\cdot\cos\left[\left(S_1-S_2\right)/\hbar+\alpha\right]\right\}. \qquad (11\cdot25)$$

Here the first term means the action of heterogeneous magnetic field upon the magnetic moment which is of magnitude $\beta=\hbar g$ and in either direction of $\pm z$. The liquids are further acted on by the horizontal component of H in the particular relation expressed in the 2nd term of (11·25). Since this force explicitly depends on the difference of velocity *potentials* S_1-S_2, at least the original picture (that is, the fluidal motion with particular internal force depending only upon the density distribution $P(\boldsymbol{x})$) here breaks down. In order somehow to regard (11·23) as an equation for classical motion, we might impart to each S_i twofold meanings of velocity potential and of some force potential, in like manner as Bohm has done for R. Such makeshift, however, could no longer be reasonable.

Furthermore these two fluids are perfectly different from usual ones in their transformation property for rotations of coordinate axes.

The picture may become possible in exceptional case $H_\perp=0$ where spin and orbital motions are perfectly separable.

The two-fluid model, though involves serious difficulties, allows us to evaluate, e.g., mean values of various quantities. For example, as far as we regard terms $\pm\hbar gH_z$ and $\hbar\gamma/P_i$ in (11·16) and (11·17) as potential energy, these contribute to the mean value of energy, the amount:

$$\langle E_s\rangle=\hbar g\int H_z\left(P_1-P_2\right)d\boldsymbol{x}+2\int\hbar\gamma\,d\boldsymbol{x}\,,$$

which is identical with the quantum-mechanical spin energy:

$$\langle E_s\rangle_{\mathrm{QM}}=\hbar g\sum\int\psi^*\boldsymbol{\sigma}\boldsymbol{H}\psi\,d\boldsymbol{x}\,.$$

(d) Relativity

Next we consider relativistic wave equations for a particle. First we take up the spinless Klein-Gorden equation as a relativistic modification of one-particle Schrödinger equation. It is written as

$$\left\{\left(\frac{\hbar}{i}\partial_\mu-\frac{e}{c}A_\mu\right)^2+m^2c^2\right\}\psi=0\,,\qquad(\mu=1,\,2,\,3,\,0)\qquad(11\cdot26)$$

where A_μ is electromagnetic potential, and $\partial_\mu=(\nabla,\,\partial/\partial ct)$. Inserting again $\psi=R\exp(iS/\hbar)$, (11·26) transforms into

$$(\partial_\mu S-eA_\mu/c)^2+m^2c^2-\hbar^2\Box R/R=0\,,\qquad(11\cdot27)$$

$$\partial_\mu[P(\partial^\mu S-eA^\mu/c)]=0\,.\qquad(11\cdot28)$$

Now if we assume extra scaler potential field* $U'=-(\hbar^2/2)\Box R/R$, Eq. (11·27) is the classical (relativistic) Hamilton-Jacobi equation, and its velocity field is compatible with regarding the expression

$$j^\mu=P(\partial^\mu S-eA^\mu/c)/m$$

as density and current, so (11·28) means the equation of continuity. Thus we seemingly get an ensemble of classical trajectories under certain extra scaler potential determined by the quantity P, which is not the density itself in this case. As is well known, however, the density j^0/c^2 is not positive definite, so in actuality the picture of a trajectory ensemble fails. This fact reflects merely that the Klein-Gordon's wave function ψ (whose equation of motion is not of general form (11·1)) cannot be regarded as probability amplitude for a particle or for any others.

For Dirac's spinor equation as the more proper relativistic wave equation for a particle, it is impossible to apply our procedure and to derive the picture of an ensemble of classical motions, for the reasons stated in respect to non-relativistic wave equation with spin, moreover the substitution (11·15) for Dirac's spinor is not reasonable from the consideration of relativistic invariance.

In place of our procedure one may apply the procedure similar to the W.K.B. method to Dirac equation, which is based on the substitution:

$$\psi_\rho=a_\rho\exp(iS/\hbar)\,,\qquad(11\cdot29)$$

in place of (11·15). As S is taken common, S and a_ρ are in general no longer real*. This procedure may lead to the explanation of the *approximate* meaning of the picture of the (relativistic) trajectory ensemble to Dirac's wave[10].

(e) Electron field

Finally, since we know it is also possible to treat electron entirely from the standpoint of field theory, we shall investigate whether it is possible to represent a change of state of quantized electron field by an ensemble of changes of states of some 'classical electron field' just as the case of electromagnetic field.

For this purpose we take up the Schrödinger field for simplicity, first as 'classical' field. The procedure is similar to the case of vector meson stated in (b), but we shall recapitulate it. The wave equation may be derived by means of the variational principle, taking

* The extra force field is derived from this potential as $-(x/p)\nabla U'$.

$$\mathcal{L}=(i\hbar/2)(\dot{\psi}\psi^*-\dot{\psi}^*\psi)-(\hbar^2/2m)\nabla\psi^*\nabla\psi-V\psi^*\psi\,, \tag{11·30}$$

as Lagrangian density. This leads to the Hamiltonian

$$H=\int\left(\frac{\hbar^2}{2m}\nabla\psi^*\nabla\psi+V\psi^*\psi\right)d\boldsymbol{x}\,, \tag{11·31}$$

with ψ and $i\hbar\psi^*$ as canonically conjugate field variables. The quantization of this field is carried out by setting the commutation relation

$$[\psi(\boldsymbol{x}),\psi(\boldsymbol{x}')^*]=\delta(\boldsymbol{x}-\boldsymbol{x}')\,, \tag{11·32}$$

if we are to regard the particle as *Boson*.

The field may be expanded by energy eigenfunctions for one-particle problem, $u_k(\boldsymbol{x})$, as

$$\psi(\boldsymbol{x},t)=\sum_k a_k(t)\,u_k(\boldsymbol{x})\,, \tag{11·33}$$

with which is associated the commutation relation

$$[a_k,a_l^*]=\delta_{kl}\,. \tag{11·34}$$

The Hamiltonian then reduces to

$$H=\sum_k E_k a_k^* a_k\,, \tag{11·35}$$

with E_k as energy eigenvalues for the one-particle problem. Further by relations

$$\begin{cases} a_k=(q_k/\hbar+ip_k)/\sqrt{2}\,, \\ a_k^*=(q_k/\hbar-ip_k)/\sqrt{2}\,, \end{cases} \tag{11·36}$$

we transform a_k and a_k^* into Hermitian variables q_k, p_k, satisfying ordinary commutation relations:

$$[p_k,q_l]=(\hbar/i)\delta_{kl}\,. \tag{11·37}$$

Then

$$H=\sum_k(p_k^2+q_k^2/\hbar^2-1)E_k/2\,. \tag{11·38}$$

This indicates the system may again be regarded as an assembly of oscillators.

We can now apply the general procedure stated in (a): By the substitution $\Psi(q_k,t)=R\exp(iS/\hbar)$ for the state vector in its q-representation, the equation of motion for state vector is transformed into

$$\begin{cases} \dot{S}+H\left(q_k,\dfrac{\partial S}{\partial q_k}\right)-\dfrac{\hbar^2}{2R}\sum_k E_k\dfrac{\partial^2 R}{\partial q_k^2}=0\,, \\ \dot{P}+\sum_k\dfrac{\partial}{\partial q_k}\left[P\cdot E_k\dfrac{\partial S}{\partial q_k}\right]=0\,. \end{cases}$$

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* In place of our method which separates the equation into its real and imaginary parts, W.K.B. method separates the equation *approximately* according to the order in $\hbar$.

These mean as before an ensemble of classical motions of an assembly of field oscillators with extra potential $-(\hbar^2/2R)\sum_k E_k(\partial^2 R/\partial q_k^2)$. The quantum-mechanical motion of the field variable ψ for some state is represented by an ensemble of its classical motions:

$$\psi(\boldsymbol{x},\ t)=\sum_k 2^{-1/2}(q_k(t)/\hbar+i\partial S/\partial q_k)u_k(\boldsymbol{x}).$$

Now if we are to consider the particle as *Fermion*, a_k and a_k^* must satisfy the anticommutation relation, then it is impossible to define any Hermitian variables q_k, p_k satisfying ordinary commutation relations and so having continuous eigenvalues. As we thus cannot obtain what we have called coordinate representation, the picture of an ensemble of classical field motions cannot be drawn. Such a situation implies that for Fermi field whose wave function has no classical analogue on account of the exclusion principle, our formulation is not feasible in contrast to the case of Bose field treated in (b).

The situation is the same for quantum Dirac field, for which Hamiltonian is again expressible as (11·35) *including the freedom of spin*, but because of the anticommutation relation for a and a^* we cannot grasp it in such formulation.

For quantum Schrödinger field of Fermion, we could in fact carry out the procedure starting from the equivalent formulation in configuration space (see (2·12)), but for Dirac field the procedure can be carried out in neither formulation. Such a consequence may not be accidental, but is in connection with the necessary relation between spin and statistics.

Since it seems very probable that for the exact validity of the picture of an *ensemble* of *corresponding* classical motions we must be able to apply the procedure stated in (a) to the system—even if it might be possible somehow to provide the spin with some classical picture of another character,—we may conclude that the ensemble picture cannot be obtained for Fermion, by the consideration of spin or exclusion principle. Then the coherent application of Bohm's new statistical interpretation for quantum mechanics must fail for Fermions.

§ 12. Similar substitution for field variable

In order to apply our method to fields, we had to make the usual substitution for the state vector. Apart from the purpose of deducing the formulation associated with classical pictures, also it is formally conceivable to put the substitution $\psi=R\exp(iS/\hbar)$ for the wave function ψ regarded as *field variable*. Such a transformation may be of use for spinless field with single complex field variable, meaning to transform the variables from ψ and ψ^* into R (or P) and S. In quantized field these variables will become q-numbers.

The Klein-Gordon's equation is in fact to be regarded as a field equation, and so its re-expression* (11·27) and (11·28) may properly be reinterpreted in such viewpoint. On the other hand, such transformation is not applicable to real fields without charge

* These, as field equations, are derivable from the Lagrangian whose density is $\mathcal{L}=-\hbar^2(\partial_\mu R)^2-R^2(\partial_\mu S)^2-m^2c^2R^2$, for free field.

such as the electromagnetic*.

We shall now briefly consider the case of Schrödinger field. Its Lagrangian density (11·30) is written, by the transformation

$$\begin{cases} \psi = P^{1/2} \exp(iS/\hbar), \\ [\psi^* = \exp(-iS/\hbar) P^{1/2}], \end{cases} \tag{12·1}$$

as

$$\mathcal{L} = -P\left(\dot{S} + \frac{1}{2m}(\nabla S)^2 + V + \frac{\hbar^2}{8m}\frac{(\nabla P)^2}{P^2}\right), \tag{12·2}$$

and Eqs. (2·10) and (2·11) are really derivable as the Euler's equation for this Lagrangian.

From (12·2) the canonical momenta conjugate to S and P are $\pi_S = -P$, and $\pi_P = 0$ respectively, so we have Hamiltonian density:

$$\mathcal{H} = -P\dot{S} - \mathcal{L} = P\left\{\frac{1}{2m}(\nabla S)^2 + V + \frac{\hbar^2}{8m}(\nabla P)^2/P^2\right\}. \tag{12·3}$$

This, if regarded as a functional of S and $\pi_S = -P$, with P and π_P eliminated, again reproduces (2·10) and (2·11) as its Hamilton equations.

From (12·2) the energy-momentum tensor may also be calculated: For example, the momentum density is obtained as $\boldsymbol{G} = P\nabla S$, in harmony with the previous picture**, as well as (12·3) for energy.

Now we may quantize the Schrödinger field formally in terms of S and P, by setting the commutation relation: ***

$$[S(x), P(x')] = (\hbar/i)\,\delta(x - x'), \tag{12·4}$$

just as we have done so by (11·21), again assuming the particle as Boson.

This way of quantization is analogous to the quantization of irrotational motion of fluid, which has been carried out by Landau[11] in connection with the problem of liquid He II, and which considered to give rise to photon corresponding to longitudinal waves. Our quantized Schrödinger field differs from quantized flow of usual liquid for its peculiar 'pressure' term, yet it might have some connection with He problem as it corresponds to an assembly of Bose particles****.

As the result of quantization, P and S no longer hold the bearing concerning the picture of the trajectory ensemble.

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* Similar procedure is still applicable to each field oscillator of electromagnetic field which is a complex fourier component representing a propagating wave; namely we transform the field variables from q_λ, p_λ in § 11, (b) into P_λ, S_λ, such that $cp_\lambda + ikq_\lambda = (2\hbar ck)^{1/2} P_\lambda \exp(iS_\lambda/\hbar)$.

** If we take P and S as field variable and its conjugate momentum respectively, as Bohm did, field momentum density is calculated as $G = -S\nabla P$, not in accordance with the picture.

*** Rigorously speaking, the definition of S as q-number through (12·1) is not feasible, further that of P^{-1} appearing in (12·3) and (2·10) is not sufficiently evident.

**** It is to be noted that we here treated for simplicity the problem neglecting mutual interaction between particles.

§ 13. Possible generalization of Schrödinger equation

The expression of Schrödinger wave equation in terms of amplitude and phase has corresponded to the hydrodynamical picture or the statistical picture, neither of which can be taken as real, as we have already seen; yet by the help of this analogy we may formally suggest a possible way of generalization of the Schrödinger equation different from the one suggested by Bohm.

As was remarked in § 3 the Schrödinger equation corresponds to an irrotational motion of compressible fluid with special 'pressure' potential. Suppose we now generalize this equation into the form corresponding to more general flow including the rotational*. We then take as fundamental equations the Euler's equation itself with special 'pressure' potential:

$$m\left\{\frac{\partial \boldsymbol{v}}{\partial t}+(\boldsymbol{v}\nabla)\boldsymbol{v}\right\}=-\nabla\left(V-\frac{\hbar^2}{2m}\frac{\Delta R}{R}\right), \tag{3·3}$$

together with continuity equation:

$$\dot{P}+\operatorname{div}(P\boldsymbol{v})=0\,. \tag{3·2}$$

We thus represent a 'quantum-mechanical state' of a particle not by the Schrödinger's ψ (i.e. by P and S) but by P and $\boldsymbol{v}$, satisfying (3·3) and (3·2), which can no longer be combined into single equation for a complex variable. From the viewpoint of the statistical picture, this means to extend the condition for an *elementary ensemble*, and the physical meaning of P and $\boldsymbol{v}$ must be considered the same as in the original statistical picture.

Such generalization requires to violate the general concept of quantum mechanics; but, instead, we can consider Eqs. (3·3) and (3·2) not as equations for a particle, but as field equations. Such field equations may not be so plausible, being non-linear and non-relativistic, yet they might possibly serve as some model, taking into consideration that, in such a field, since the irrotational form of flow corresponds to the translational motion of structureless particle, the rotational flow may imply some other things. To examine this point the field should be quantized. The quantization of ordinary fluidal motion, including rotational flow, has been suggested by Landau[11] as was mentioned in § 12. We shall briefly sketch the method.

We set up, as the generalization of (12·4), the commutation relation

$$[\boldsymbol{v}(\boldsymbol{x}), P(\boldsymbol{x}')]=(\hbar/im)\nabla\delta(\boldsymbol{x}-\boldsymbol{x}'),$$

again considering Bose particles. Further, following Landau, we set up**

$$[v_i(\boldsymbol{x}),\ v_j(\boldsymbol{x}')]=(\hbar/im)\ \delta(\boldsymbol{x}-\boldsymbol{x}')P^{-1}(\operatorname{curl}\boldsymbol{v})_k\,.$$

As Hamiltonian, we take the expression for energy:

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* When magnetic field is present, Schrödinger equation corresponds to certain rotational flow, which is not however a general one but with potential for the quantity $\boldsymbol{v}+(e/mc)\boldsymbol{A}$ (see § 3).

** (i,j,k) means an even permutation of (x,y,z).

$$H=\int\left\{\frac{m}{2}\boldsymbol{v}P\boldsymbol{v}+PV+\frac{\hbar^2}{8m}(\nabla P)^2P^{-1}\right\}d\boldsymbol{x}\,.$$

It is then shown that the equations of motion (3·3) and (3·2) are given each in standard form :

$$\dot{\boldsymbol{v}}=(i/\hbar)[H,\boldsymbol{v}]\,,\qquad \dot{P}=(i/\hbar)[H,P]\,.$$

Now there exist the states which always satisfy curl $\boldsymbol{v}=0$ everywhere, since curl $\boldsymbol{v}$ commutes with H when it vanishes. Such states just cover those of Schrödinger field (stated in § 12). The lowest state of vortex motion and the spectrum near it have been conjectured by Landau in terms of so-called 'roton.' Corresponding to this we might have something like spin with excited states in our case, but it may be difficult to analyse the vortex motion, and we cannot here enter into this problem.

§ 14. Singular ensembles with kernel property, etc.

Apart from the difficulties in its interpretation or the restriction on its applicability, our procedure has enabled an alternative formulation of quantum mechanics (especially in respect to equation of motion and stationary state problems) provided with certain classical pictures. One must be able to treat various problems according to this formulation. We shall, in this section, construct special singular solutions on this formulation, and find a connection between this formulation and the Feynman's one.

Now, this formulation has the advantage that it can utilize the classical picture, nevertheless, the peculiar quantum-theoretical potential $-(\hbar^2/2m)\Delta R/R$ exerts so essential influence that in fact it is generally more difficult to find the solution along this way, reflecting that the formulation is constructed with the non-linear, simultaneous equations unlike the original Schrödinger wave mechanics.

It is, however, usefull for such distributions where $\Delta R/R=0$, because in this case quantum-theoretical potential really vanishes and we have the picture of an ensemble of *purely* classical trajectories. Also it is possible to proceed along successive approximation in which quantum-theoretical potential is first neglected (see § 15).

We take up in this section spatially uniform distributions which of course satisfy $\Delta R/R=0$. Such an ensemble must therefore fulfil three simultaneous relations :

$$\begin{cases} \nabla P=0\,, & (14\cdot1)\\ \dot{S}+\dfrac{1}{2m}(\nabla S)^2+V=0\,, & (14\cdot2)\\ \dot{P}+P\Delta S/m=0\,. & (14\cdot3) \end{cases}$$

Here Eq. (14·2) involves only S as unknown function, but S must further satisfy*

$$\nabla(\Delta S)=m\nabla\,\mathrm{div}\,\boldsymbol{v}=0\,, \qquad (14\cdot4)$$

* For such solution be allowable *exactly*, it is sufficient that V is a polynomial below 2nd power in $\boldsymbol{x}$.

so that (14·1) and (14·3) might not contradict each other. If this is the case, P is determined from (14·3) as

$$P=\text{const.}\exp\Big(-\int \operatorname{div} \boldsymbol{v}\, dt\Big). \tag{14·5}$$

Now, to solve (14·2) means to obtain an action function for purely classical motions. On the other hand the classical trajectory $\boldsymbol{x}(t)$, which starts from a point $\boldsymbol{x}_0$ at time $t=0$ and reaches $\boldsymbol{x}$ at t, can be determined by the variational equation:

$$\int_0^t L(\dot{\boldsymbol{x}}(t), \boldsymbol{x}(t))\, dt=\min., \qquad (\boldsymbol{x}(0)=\boldsymbol{x}_0, \qquad \boldsymbol{x}(t)=\boldsymbol{x}),$$

the minimum value of which means the action for this classical motion, i.e.,

$$S(\boldsymbol{x}t, \boldsymbol{x}_0 0)=\Big[\int_0^t L(\dot{\boldsymbol{x}}(t), \boldsymbol{x}(t))\, dt\Big]_{\min}. \tag{14·6}$$

Here the Lagrangian L is known, for the case under consideration, to be

$$L(\dot{\boldsymbol{x}}, \boldsymbol{x})=\frac{m}{2}\dot{\boldsymbol{x}}^2-V(\boldsymbol{x}). \tag{14·7}$$

The action function $S(\boldsymbol{x}t, \boldsymbol{x}_0 0)$, given by (14·6), regarded as a function of $\boldsymbol{x}$ and t, fixing $\boldsymbol{x}_0$, is a singular solution of (14·2), such as to correspond to the trajectories starting from a fixed point $\boldsymbol{x}_0$ initially with any velocity. Such S, if satisfies (14·4), gives, combined with (14·5), a possible (elementary) ensemble (i.e., a solution of Schrödinger equation).

Really this is the case in general in the *infinitesimal neighbourhood* of space-time point $(\boldsymbol{x}_0, 0)$. It is because we have, in such space-time region, by (14·6) and (14·7),

$$S(\boldsymbol{x}t, \boldsymbol{x}_0 0)\simeq \frac{m}{2t}(\boldsymbol{x}-\boldsymbol{x}_0)^2-\frac{t}{2}(V(\boldsymbol{x})+V(\boldsymbol{x}_0)) \tag{14·8}$$

$$\simeq \frac{m}{2t}(\boldsymbol{x}-\boldsymbol{x}_0)^2-t\Big\{\frac{1}{2}(\boldsymbol{x}-\boldsymbol{x}_0)(\nabla V)_0+V(\boldsymbol{x}_0)\Big\}, \tag{14·8$'$*}$$

and so

$$\boldsymbol{v}=\nabla S/m=\frac{\boldsymbol{x}-\boldsymbol{x}_0}{t}-\frac{t}{2m}(\nabla V)_0, \quad \operatorname{div}\boldsymbol{v}=3/t. \tag{14·9}$$

Then from (14·5) and (14·9) we get

$$P=\text{const.}\, t^{-3}. \tag{14·10}$$

We have thus found that the spatially uniform ensemble of purely classical trajectories starting from space-time point $(\boldsymbol{x}_0, 0)$ with various velocities, is a possible (elementary) ensemble in the neighbourhood of this space-time point.

This ensemble has been obtained as a very particular solution, nevertheless it possesses the following universal significance: The wave function corresponding to this ensemble,

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* Expression (14·8)′ is identical with (14·8) in our approximation which neglects terms of order of $t(\boldsymbol{x}-\boldsymbol{x}_0)^2$.

$$K(\boldsymbol{x}t, \boldsymbol{x}_0 0) = P(t)^{1/2} e^{(i/\hbar) S(\boldsymbol{x}t; \boldsymbol{x}_0 0)} \tag{14·11}$$

$$= \text{const. } t^{-3/2} \cdot \exp \frac{i}{\hbar} \left[\frac{m}{2t} (\boldsymbol{x}-\boldsymbol{x}_0)^2 - t \left\{ \frac{1}{2} (\boldsymbol{x}-\boldsymbol{x}_0) (\nabla V)_0 + V(\boldsymbol{x}_0) \right\} \right], \tag{14·11}'$$

is the transformation kernel to produce the wave function $\psi(\boldsymbol{x}, t)$ *at infinitesimally later instant* from its initial form $\psi(\boldsymbol{x}, 0)$, by the relation:

$$\psi(\boldsymbol{x}t) = \int K(\boldsymbol{x}t, \boldsymbol{x}_0 0)\, \psi(\boldsymbol{x}_0 0)\, d\boldsymbol{x}_0 . \tag{14·12}$$

To see this, first we note that the expression (14·12) satisfies the Schrödinger equation for small t. It is because in the neighbourhood of $\boldsymbol{x}_0$, $K(\boldsymbol{x}t, \boldsymbol{x}_0 0)$ itself satisfies the wave equation as we have above deduced, and on the other hand the region where $\boldsymbol{x}-\boldsymbol{x}_0$ is not small makes no contribution to the integral of (14·12) as the factor $\exp\left[(im/2\hbar t)(\boldsymbol{x}-\boldsymbol{x}_0)^2\right]$ in K oscillates rapidly due to the smallness of t. In the second place we note that when $t \to 0$ the expression (14·12) tends to const. $\psi(\boldsymbol{x}, 0)$ because* when $t \to 0$

$$\lim_{t\to 0} K(\boldsymbol{x}t, \boldsymbol{x}_0 0) = \lim_{t\to 0} \text{const. } t^{-3/2} \cdot \exp\left[\frac{i}{\hbar} \frac{m}{2t} (\boldsymbol{x}-\boldsymbol{x}_0)^2 \right] = \text{const. } \delta(\boldsymbol{x}-\boldsymbol{x}_0). \tag{14·13}$$

Thus the quantity $K(\boldsymbol{x}t, \boldsymbol{x}_0 0)$, whose amplitude is spatially uniform and whose phase is the action of the classical trajectory from $(\boldsymbol{x}_0 0)$ to $(\boldsymbol{x}t)$, means the kernel of the Schrödinger wave function to infinitesimally later instant; but this is just the Huygens' principle for the development of Schrödinger wave, which has clearly been expressed by Feynman.[1]**

We shall now reproduce the above argument in somewhat more intuitive form. First, taking the gradient of (14·2), we get the classical Newton's equation:

$$m \frac{d\boldsymbol{v}}{dt} = -\nabla V. \tag{14·14}$$

A classical trajectory $\boldsymbol{x}_t$, $\boldsymbol{v}_t$ (particle position and velocity at time t) are expanded, for small t, as

$$\begin{cases} \boldsymbol{v}_t \simeq \boldsymbol{v}_0 + t\dot{\boldsymbol{v}}_0, & (14·15) \\ \boldsymbol{x}_t \simeq \boldsymbol{x}_0 + t\boldsymbol{v}_0 + \dfrac{t^2}{2}\dot{\boldsymbol{v}}_0. & (14·16) \end{cases}$$

Suppose we vary the initial conditions of motion $(\boldsymbol{x}_0, \boldsymbol{v}_0)$, then (14·15) and (14·16) represent trajectories of number of ∞^6, from which we pick up a collection of trajectories of number of ∞^3, by fixing $\boldsymbol{x}_0$. They are the motions passing the point $\boldsymbol{x}_0$

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* Note that, $\lim_{t\to 0}\left(\frac{i\hbar t}{m}\right)^{-3/2} \exp\left(\frac{i}{\hbar}\frac{m\boldsymbol{x}^2}{2t}\right) = \lim_{t\to 0} h^{-3} \int \exp\left[-\frac{i}{\hbar}\left(\boldsymbol{p}\boldsymbol{x} + \frac{\boldsymbol{p}^2}{2m} t\right)\right] d\boldsymbol{p} = \delta(\boldsymbol{x})$.

** Feynman's procedure corresponds to first postulating (14·12) with (14·11) and (14·6) [or(14·8)], and then proving its satisfying Schroedinger equation, together with (14·10), by means of Taylor expansion in t.

initially with any velocity, and they construct a definite velocity field $v(x, t)$ which is obtained by eliminating v_0 and $\dot{v}_0$ from (14·14), (14·15) and (14·16), as

$$x = x_0 + tv(x, t) + (t^2/2m)(\nabla V)_0 , \qquad (14\cdot17)$$

but this is just identical with (14·9). We may therefore readily construct the velocity potential S for this velocity field so as to satisfy (14·2), again reaching (14·8)′.

Moreover in this way we shall also be able to show that this velocity potential S means the phase of the transformation kernel. It is as follows. Eq. (14·16) combined with (14·14) is written as

$$x_t = x_0 + tv_0 - \frac{t^2}{2m}(\nabla V)_0 , \qquad (14\cdot18)$$

which must also be valid in quantum mechanics as a q-number relation. Then the transformation function $K(x_0 0, xt)$ from the representation making x_0 diagonal to the one making x_t diagonal, has to satisfy the equation gained in the following way: In (14·18) we replace v_0 by $(\hbar/mi)\nabla_0$, and then operate this result on K, thus,

$$\left\{x_0 + \frac{t}{m}\frac{\hbar}{i}\nabla_0 - \frac{t^2}{2m}(\nabla V)_0\right\} K = xK . \qquad (14\cdot19)$$

This equation, when re-expressed for the phase S of K $[K = \text{const.}\exp(iS/\hbar)]$, turns back into,

$$\text{Eq. (14·18) with } v_0 \text{ replaced by } \nabla_0 S(x_0 0, xt)/m . \qquad (14\cdot20)$$

Further, taking into account the property:

$$K(x_0 0, xt) = K(xt, x_0 0)^*, \qquad \therefore\ S(x_0 0, xt) = -S(xt, x_0 0), \qquad (14\cdot21)$$

(14·20) is also written as

$$\text{Eq. (14·17) with } v \text{ regarded as } \nabla S(x', x_0 0)/m , \qquad (14\cdot22)$$

which is just the relation (14·9). Then, integrating (14·22) by the help of (14·21), we again reach (14·8)′. From the above parallelism the kernel property of S is quite clear.

Next we consider special cases when the S function, which corresponds to the ensemble of classical trajectories passing a space-time point $(x_0, 0)$ with any velocity, fulfills the condition (14·4) over a finite space-time region, and so exact solution may be obtained for finite time interval.

Since such an ensemble must tend to agree with (14·8) and (14·10) in the neighbourhood of $(x_0, 0)$, it has the property of kernel for small t, accordingly must also have for finite t.

To satisfy (14·4), considering, for simplicity, one dimensional cases, the S-function must be quadratic in x, that is,

$$S = s_0 x^2 + 2s_1 x + s_2 . \qquad (14\cdot23)$$

On the other hand this S-function must satisfy (14·2), and this fact requires V to be quadratic in x. Suppose now the solutions of the Newton's equation are obtained in linear form in initial values x_0 and v_0, such that

$$x=fv_0+gx_0+h\,, \tag{14·24}$$

where f, g, h are functions of t alone. Then we readily find the S-function corresponding to the classical trajectories passing $(x_0, 0)$ to be really quadratic in x such as (14·23) with the relations $s_0=(m/2)(\dot{f}/f)$, etc., accordingly we have

$$P=\text{const.}\, f^{-1}. \tag{14·25}$$

Example 1. *Oscillator*[12]

For oscillator having potential $V=m\omega^2x^2/2$, the classical action function connecting two space-time points $(x_0 0)$, (xt) can easily be found to be

$$S=\frac{m\omega}{2\sin\omega t}\{(x^2+x_0^2)\cos\omega t-2xx_0\}, \tag{14·26}$$

which is certainly quadratic in x. The Newton's solutions (14·24) takes the form:

$$\left.\begin{aligned} x&=v_0\sin\omega t/\omega+x_0\cos\omega t\,,\\ v&=v_0\cos\omega t-x_0\omega\sin\omega t\,. \end{aligned}\right\} \tag{14·27}$$

and so

Then by (14·25),

$$P=\text{const}/\sin\omega t\,. \tag{14·28}$$

Eqs. (14·26) and (14·28) give the kernel for finite time transformation by $K(xt, x_0 0)=P^{1/2}\exp(iS/\hbar)$.

Similarly we can obtain such kernel for forced oscillator which is subject to any perturbing force $\gamma(t)$.

Example 2. *Motion under Uniform Magnetic Field*

For uniform distribution Eq. (3·9) reduces to purely classical Newton's equation:

$$m\frac{d\boldsymbol{v}}{dt}=\frac{e}{c}[v\times H]\,.$$

As is well known, classical trajectories under uniform magnetic field are the circular motions* with constant angular velocity, $\omega=eH/mc$, that is,

$$\left\{\begin{aligned} \zeta&=\zeta_0 e^{-i\omega t},\\ \xi&=(i\zeta_0/\omega)(e^{-i\omega t}-1)+\xi_0\,, \end{aligned}\right. \tag{14·29}$$

where $\zeta=v_x+iv_y$ and $\xi=x+iy$ are complex velocity and position respectively; ζ_0 and ξ_0 their initial values.

The velocity field corresponding to the trajectories passing a fixed space-time point

* We consider the motion for simplicity only in the plane perpendicular to $\boldsymbol{H}$.

$(\xi_0, 0)$ with arbitrary velocity, is obtained as before by eliminating ζ_0 from (14·29), as

$$\zeta(\xi, t) = -i\omega(\xi - \xi_0)/(1 - e^{i\omega t}). \tag{14·30}$$

This satisfies the condition (14·4), and leads to

$$\begin{cases} P = \text{const.}/(1-\cos\omega t), \\ S(\xi t, \xi_0 0) = \dfrac{m\omega}{4}\left\{\dfrac{\sin\omega t}{1-\cos\omega t}\,|\xi-\xi_0|^2 + i(\xi_0\xi^* - \xi_0{}^*\xi)\right\}. \end{cases}$$

Combining P and S, we obtain the kernel exact for finite time interval as in the case of oscillator.

Next we shall briefly consider the ensemble reciprocal to what we have treated so far, the ensemble of classical trajectories which start from any point in space initially with a fixed momentum $\boldsymbol{p}_0$. The momentum field constructed by such trajectories, when t is infinitesimally small, is simply

$$\boldsymbol{p}(\boldsymbol{x}, t) = \nabla S = \boldsymbol{p}_0 - t\nabla V, \tag{14·31}$$

which gives $\operatorname{div}\boldsymbol{p} = -t\Delta V$. Therefore, if ΔV is space independent*, (14·31) leads to a possible ensemble. That is,

$$P = \text{const.}, \qquad S = \boldsymbol{p}_0\boldsymbol{x} - (\boldsymbol{p}_0^2/2m + V)t. \tag{14·32}$$

For some cases we can also obtain the similar ensemble as an exact solution for finite t. For example, again for oscillator, we obtain, by eliminating x_0 from (14·27) with v_0 fixed,

$$v(x, t) = (v_0 - x\omega\sin\omega t)/\cos\omega t,$$

and, from this

$$\begin{cases} P = \text{const.}/\cos\omega t, \\ S = (p_0 x - E'\sin\omega t/\omega)/\cos\omega t, \qquad (E' \equiv p_0^2/2m + V). \end{cases}$$

Finally, it is sufficient for the validity of purely classical trajectories only that $\Gamma(\Delta R/R) = 0$. This is satisfied by real functions** which have the property of the energy eigenfunction in free space such as plane waves:

$$R = a\cos(\boldsymbol{k}\boldsymbol{x} + \alpha), \qquad (-(\hbar^2/2m)\Delta R/R = \hbar^2\boldsymbol{k}^2/2m), \tag{14.33}$$

or spherical waves:

$$R = b\sin kr/r, \quad \text{etc}; \quad (r = |\boldsymbol{x} - \boldsymbol{x}_0|), \tag{14·34}***$$

where a, $\boldsymbol{k}$, α, b, and $\boldsymbol{x}_0$ may still depend on t. We shall not be concerned in these cases any further here.

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* For this, it is sufficient that V be a polynomial of below 2nd power in $\boldsymbol{x}$. Such condition is required because we consider now t small but $\boldsymbol{x}$ in all space in contrast to the case of (14·8).

** We need not necessarily adhere to the assumption $R \geqq 0$.

*** Solutions $R = b\cos kr/r$ (including b/r for $k = 0$) means another singular distribution which may be also allowable.

§ 15. 'W.K.B. procedure', etc.

We have taken up in the last section singular, non-stationary, but spatially uniform ensembles, in which quantum-theoretical potential *really* vanishes, and which, by certain superposition, built up the solution for small (or finite) time interval.

Somewhat analogous procedure is the 'W.K.B. method,' in which the quantum-theoretical potential is first *neglected* from the reason that it is of 2nd order in $\hbar$, accordingly in this stage of approximation the picture of the ensemble of *purely* classical trajectories gets again valid. This means the geometrical optics approximation, and is taken as the start of further approximation. In contrary to the kernel method, this procedure is useful especially in stationary state problems. In this case such approximate solutions, when suitably superposed, may construct a better approximation, say from the ground of variational principle.

This procedure is suitable to clarify the correspondence-theoretical significances of the picture of the old quantum theory, into which we do not however enter here.

Lastly as another use of our formulation, we shall point out the problem of *wave* of the fluid with its peculiar 'pressure potential' in our hydrodynamical picture.*

We have treated various aspects of our subject but not fully developed the analysis in some points, which we want to carry out in future work.

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References

1) R. P. Feynman, Rev. Mod. Phys. **20** (1948), 367.
2) D. Bohm, Phys. Rev. **84** (1952), 166, 180.
3) L. de Broglie, *Introduction à l'étude de la Mécanique ondulatoire* (Hermann, Paris, 1930). See also, E. Madelung, ZS. Phys. **40** (1926), 332; E. H. Kennard, Phys. Rev. **31** (1928), 876.
4) The present author came to this formulation in course of his analysis in the correspondence-theoretical relations between quantum mechanics and classical theory. In this connection, see T. Takabayasi, 'Charge-Cloud Atom' ('Shizen' No. 7, 9, 11 (1951), No. 3 (1952)), 'On the Concepts of Oscillator and Charge-Cloud' (Jour. of History of Science, Japan, Oct. 1951).
5) See, e. g., M. Taketani, 'Kagaku' **12** (1942), 807; S. Sakata, Prog. Theor. Phys. **2** (1947), 145.
6) For relativistic quantum mechanics, on the other hand, it is to be recalled of that Sakata has given insights into the present stage of the theory that "the Tomonaga-Schwinger formalism is considered in some way to be an *abstract* formalism, behind which the physical *model* of the elementary particles lies hidden." See, S. Sakata and H. Umezawa, Prog. Theor. Phys. **5** (1950), 682.
7) Similar comment was briefly given by H. Yukawa ('Kagaku' **21** (1951), 410).
8) See, e.g., G. Wentzel, *Einführung in die Quantentheorie der Wellenfelder* (Wien, 1943), § 12.
9) See, S. Nakajima, K. Tomita and T. Usui, Phys. Rev. **78** (1950), 768. The equal allotment is natural in our case because of the symmetricity between both spin states, but may be somewhat arbitrary in He II problem.

* See appendix B.

10) W. Pauli, *Die Allgemeinen Prinzipien der Wellenmechanik* (1933), B. Ziff. 4.
11) L. Landau, Jour. Phys. U.S.S.R. **5** (1941), 71.
12) Compare with the case by Feynman's method (see his lecture, *Quantum Electrodynamics* (1950) p. 13).

Appendix

A. Stress tensor in the hydrodynamical picture

In hydrodynamical picture we have considered merely the pressure potential $-(\hbar^2/2m)\Delta R/R$ so far. This is however identical with assuming certain *stress tensor*. From (3·3) and (3·2) we get

$$m\frac{\partial}{\partial t}(Pv_i)+m\sum_k\frac{\partial}{\partial x_k}(Pv_iv_k)=PK_i+\sum_k\frac{\partial}{\partial x_k}\sigma_{ik}, \tag{A·1}$$

where $K_i=-\partial V/\partial x_i$, and

$$\sigma_{ik}=\frac{\hbar^2}{2m}\left(R\frac{\partial^2 R}{\partial x_i\partial x_k}-\frac{\partial R}{\partial x_i}\frac{\partial R}{\partial x_k}\right)=\frac{\hbar^2}{2m}P\frac{\partial^2(\log R)}{\partial x_i\partial x_k}. \tag{A·2}$$

This showes that the motion can just be pictured as that of fluid with (symmetric) stress tensor σ_{ik}, and that the influence of quantum mechanics is regarded as introducing this '*quantum-theoretical*' *stress* (in addition to considering an irrotational fluidal motion). The *force* naturally remains the same as before, that is,

$$\sum_k\frac{\partial}{\partial x_k}\sigma_{ik}=P\frac{\partial}{\partial x_i}\left(\frac{\hbar^2}{2m}\frac{\Delta R}{R}\right). \tag{A·3}$$

In this viewpoint the peculiarities of our hydrodynamics present itself in the stress tensor rather than in the divergent pressure potential. The normal components σ_{ii} of the stress may be *tension-like* ($\sigma_{ii}>0$) as well as pressure-like ($\sigma_{ii}<0$). Also the mean pressure

$$\bar{p}_r=-\frac{1}{3}\operatorname{spur}\sigma=\frac{\hbar^2}{6m}((\nabla R)^2-R\Delta R)$$

may be negative. Further, the *shearing components*, not generally vanishing, depend only upon the density distribution but not upon the velocity field, so that the flow is dissimilar to *viscous* one and can persists to be irrotational.

The condition for perfect fluid hydrodynamics

$$\sigma_{ij}=-p_r\delta_{ij}$$

is satisfied only by the *Gaussian distribution*:

$$P=\text{const.}\exp(-ar^2),\quad (r=|\boldsymbol{x}-\boldsymbol{x}_0|)$$

with $p_r=(a\hbar^2/2m)P$.

For a little more general distribution $P=\text{const.}\exp(-ar^n)$, it is easily verified that there acts in the directions perpendicular to radius always a pressure; and in the radial direction a tension for $n<1$, and a pressure for $n>1$ which gets equal to the former pressure in mangitude for $n=2$ as was above stated.

B. Sound wave in the fluid of the hydrodynamical picture

We consider the motion of the fluid which gives rise to slight deviation from the normal state of rest in free space, $R=\text{const}(=R_0)$, $\boldsymbol{v}=0$. In this case, inserting

$$R=R_0(1+\rho), \quad |\rho| \ll 1, \tag{B·1}$$

and neglecting the term $(\nabla S)^2/2m=m\boldsymbol{v}^2/2$ because of the smallness of $\boldsymbol{v}$, we can simplify the original simultaneous equations (3·5) and (3·2) and thus bring back into the linear form

$$\dot{S}+V-\frac{\hbar^2}{2m}\Delta\rho=0\,, \tag{B·2}$$

$$\dot{\rho}+\frac{1}{2m}\Delta S=0\,. \tag{B·3}$$

Further assuming $V=0$, and putting $S/\hbar=s$, these equations are reduced to the symmetric form

$$\dot{s}-a\Delta\rho=0\,, \tag{B·2′}$$

$$\dot{\rho}+a\Delta s=0\,. \qquad (a\equiv\hbar/2m) \tag{B·3′}$$

They are identical with the real and imaginary part equations for the Schrödinger equation in free space $\dot{\psi}-ia\Delta\psi=0$, derived by the substitution $\psi=\text{const}+\text{const}(\rho+is)$. This is because

$$R_0(1+\rho)e^{is}\simeq R_0(1+\rho)(1+is)\simeq R_0(1+\rho+is)$$

for small ρ and s.

From (B·2′) and (B·3′) we get

$$\begin{cases}\ddot{s}+a^2\Delta\Delta s=0\,,\\ \ddot{\rho}+a^2\Delta\Delta\rho=0\,,\end{cases} \tag{B·4}$$

which mean the equation for the 'sound wave' in our fluid, replacing the equation

$$\ddot{S}-\beta^2\Delta S=0, \quad (\beta=dp_r/d(mP)) \tag{B·5}$$

for usual sound.

Simple plane wave solutions for (B·2′) and (B·3′) are

$$\begin{cases} s=\gamma\sin\xi_\pm\,, & \rho=\pm\gamma\cos\xi_\pm\,, & (\boldsymbol{v}=\boldsymbol{v}_0\cos\xi_\pm)\,,\\ s=\gamma\cos\xi_\pm\,, & \rho=\mp\gamma\sin\xi_\pm\,, & (\boldsymbol{v}=-\boldsymbol{v}_0\sin\xi_\pm)\,;\end{cases} \tag{B·6}$$

where $\xi_\pm=\boldsymbol{k}\boldsymbol{x}\mp ak^2t$, and $\boldsymbol{v}_0=(\hbar\boldsymbol{k}/m)\gamma$. They show that the wave must be *longitudinal* as in usual fluid, but that the phase velocity $u=ak$ depends on k unlike the case of usual fluid where $u=\beta$. For (B·1) we require that $|\gamma|\ll 1$ ($|\gamma|=v_0/2u$ meaning half of 'Mach's number'); moreover this condition is just what gurantees the legitimacy of neglecting the v^2-term in (B·2). These circumstances are similar to the case of usual sound.

For example, one of sound waves thus obtained, the first of (B·6), corresponds to the wave function

$$\psi = 1 + \gamma e^{i\xi_+} \simeq R_0 (1 + \gamma \cos \xi_+) \, e^{i\gamma \sin \xi_+}, \tag{B·7}$$

which is not any eigenstate for momentum nor for energy.

For sound waves in general cases where V exists, we cannot start from (B·2) and (B·3), because sound waves correspond to slight deviations from a normal state of rest, which is identical with a real eigenstate for energy and is defined by $R = R_0$ and $v = 0$, where R_0 satisfies

$$-(\hbar^2/2m) \Delta R_0/R_0 + V = E \, .$$

We can, however, obtain the equations which replace (B·2′) and (B·3′) still in linear and symmetrical form

$$\begin{cases} \dot{s} - \alpha [2 (\nabla R_0/R_0) \nabla \rho + \Delta \rho] = 0 \, , \\ \dot{\rho} + \alpha [2 (\nabla R_0/R_0) \nabla s + \Delta s] = 0 \, , \end{cases} \tag{B·8}$$

where ρ is defined by (B·1) as before, and $s = (S + Et)/\hbar$.

C. Hartree's approximation

For simplicity let us consider a two-electron system. Its quantum-mechanical motion is described in our formulation by an ensemble of trajectories in the configuration space under the action of external potential $V(x_1) + V(x_2)$, Coulomb repulsion $e^2/|x_1 - x_2|$ and the quantum-theoretical potential $-(\hbar^2/2mR)(\Delta_1 R + \Delta_2 R)$, as we have seen in § 2. But corresponding to the Hartree's independent orbital approximation, we reduce the picture by assuming the separation of variables:

$$R(x_1, x_2) = R_1(x_1) \cdot R_2(x_2), \quad S(x_1, x_2) = S_1(x_1) + S_2(x_2).$$

Then the motion of the first electron is pictured as an ensemble of trajectories in real space under the action of quantum-theoretical potential $-(\hbar^2/2m) \Delta R_1/R_1$ due to its own cloud, and the Coulomb potential $e^2 \int P_2(x_2) dx_2 / |x_1 - x_2|$ due to the cloud of the 2nd electron, and vice versa. It is noticeable that the cloud acts upon its own particle 'hydrodynamically' whereas upon the other particle electrostatically.

Note added in proof: Formulation of the second quantization in hydrodynamical form more strict than what we stated in § 12 has recently been attempted by Nishiyama (Prog. Theor. Rhys. **7** (1952), 417) in terms of R, Ψ, and Ψ^* (which correspond to $P^{1/2}$, $e^{iS/\hbar}$, and $e^{-iS/\hbar}$ in (12·1) respectively), introducing the velocity operator by

$$v = \frac{\hbar}{2mi} (\Psi^* \nabla \Psi - \nabla \Psi^* \cdot \Psi).$$

It is noticeable that this velocity field involves the rotational part:

$$(\text{curl } v)_i = \frac{\hbar}{mi} \left(\frac{\partial \Psi^*}{\partial x_j} \frac{\partial \Psi}{\partial x_k} - \frac{\partial \Psi^*}{\partial x_k} \frac{\partial \Psi}{\partial x_j} \right).$$

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Realization of Special Contact Transformations with Static Electromagnetic Fields in Vacuo

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Necessary conditions for two contact transformations, i.e. coordinate-coordinate transformation and momentum-coordinate transformation are obtained with static electromagnetic fields in vacuo. A velocity-coordinate transformation is shown to be impossible. An example of electromagnetic field allowing the two contact transformations is given.

§ 1. Introduction

Concerning the invention and design of energy spectrometer, mass spectrometer, oscillator and accelerator, physical intuition alone seems to have been playing le premier role enslaving mathematics in the serfdom of an aberration computer.

These instruments perform mathematically contact transformations of some specified characters between initial and final variables. So there appears the problem to find out a dynamical system which performs a specified contact transformation.

If a contact transformation $(a_r, b_r) \rightarrow (x_r, y_r)$ is realizable with a dynamical system defined by its Hamiltonian $H(x_r, y_r)$ not involving the time, the transformation must leave the Hamiltonian invariant, since the Hamiltonian is an integral of the equation of motion.

The above property of contact transformation is a guide to lead us in searching an appropriate dynamical system.

In this paper are considered two contact transformations:

1) the coordinate-coordinate transformation in which final coordinates of a particle depend upon only initial coordinates of the particle,

2) the momentum-coordinate transformation in which final coordinates depend upon initial momenta alone.

If the momentum-coordinate transformation is possible, it will be efficiently applicable to the design of momentum spectrometer if needed. The transformation is possible with a static electromagnetic field in vacuo. The momenta, however, are not the velocities, and depend upon vector potentials of field.

On the other hand, if the coordinate-coordinate transformation is possible, the transformation makes it possible to construct a perfect instrument by which all the particles emitted from any point source in any direction with any velocity will be centered at

another point. In other words, the coordinate-coordinate transformation, if possible, allows a stigmatic representation with no chromatic aberration. This transformation is possible and realizable with static electromagnetic fields in vacuo. But, the magnification ratio of a perfect instrument being unity, the transformation will be applicable not to the design of an electron microscope but to the planning of a mass spectrometer.

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§ 2. Representations of the contact transformation

If two systems of canonical variables $(a_1,\cdots, a_n, b_1,\cdots, b_n)$, $(x_1,\cdots, x_n, y_1,\cdots, y_n)$ are connected by a contact transformation, there is an invariant bilinear form

$$da_r\delta b_r - db_r\delta a_r = dx_r\delta y_r - dy_r\delta x_r\,, \tag{0}$$

where two symbols of differentiation d, δ are commutable between them and the signs of summation with respect to r are omitted.

If $2n$ variables appearing linearly in the two bilinear forms are taken as independent variables, the contact transformation takes a concise form as is well recognized. 2 cases are cited here

1) a_r, x_r being independent. We have then

$$\delta(b_r\,da_r) - d(b_r\,\delta a_r) = \delta(y_r\,dx_r) - d(y_r\,\delta x_r)$$

or

$$\delta(y_r\,dx_r - b_r\,da_r) = d(y_r\,\delta x_r - b_r\,\delta a_r)\,.$$

Hence $y_r\,dx_r - b_r\,da_r$ is a perfect differential. Therefore

$$y_r\,dx_r - b_r\,da_r = dU(x, a)\,,$$

$$y_r = \frac{\partial U}{\partial x_r}\,, \qquad b_r = -\frac{\partial U}{\partial a_r}\,.$$

2) b_r, x_r being independent,

$$y_r\,dx_r + a_r\,db_r = dV(x, b)\,,$$

$$y_r = \frac{\partial V}{\partial x_r}\,, \qquad a_r = \frac{\partial V}{\partial b_r}\,.$$

There are other types of representation corresponding to the Cayley parametrization of a symplectic matrix.[1)]

3) Taking $(x_r + a_r)/2 = u$, $(y_r + b_r)/2 = v_r$ as independent variables, and putting

$$x_r - a_r = 2f_r\,, \qquad y_r - b_r = 2g_r\,,$$

we transform (0) into

$$du_r\,\delta g_r - dg_r\,\delta u_r = dv_r\,\delta f_r - df_r\,\delta v_r\,,$$

whence we have

$$\delta(g_r\,du_r - f_r\,dv_r) = d(g_r\,\delta u_r - f_r\,\delta v_r),$$

$$g_r\,du_r - f_r\,dv_r = dF(u, v).$$

Hence we get

$$g_r = \frac{\partial F}{\partial u_r}, \qquad f_r = -\frac{\partial F}{\partial v_r},$$

$$x_r = u_r - \frac{\partial F}{\partial v_r}, \qquad a_r = u_r + \frac{\partial F}{\partial v_r},$$

$$y_r = v_r + \frac{\partial F}{\partial u_r}, \qquad b_r = v_r - \frac{\partial F}{\partial u_r}.$$

4) $(x_r - a_r)/2 = u_r$, $(y_r - b_r)/2 = v_r$ taken as independent variables.

$$x_r = u_r - \frac{\partial G}{\partial v_r}, \qquad a_r = -u_r - \frac{\partial G}{\partial v_r},$$

$$y_r = v_r + \frac{\partial G}{\partial u_r}, \qquad b_r = -v_r + \frac{\partial G}{\partial u_r}.$$

§ 3. The equation of motion

For a charged particle in a static electromagnetic field, the equation of motion can be derived from the variation principle

$$\delta \int L\,dt = 0$$

with

$$L = \frac{1}{2}\frac{dx_r}{dt}\frac{dx_r}{dt} + \frac{e}{mc}A_r(x)\frac{dx_r}{dt} - \frac{e}{m}A(x),$$

$x_r = (x_1, x_2, x_3)$	orthogonal cartesian coordinates of the particle,
$A_r = (A_1, A_2, A_3)$	vector potentials,
A	scalar potential,
m	mass of the particle,
e	charge of the particle,
c	velocity of light,
t	time.

Denoting the momentum conjugate to x_r by y_r

$$y_r = \frac{dx_r}{dt} + \frac{e}{mc}A_r,$$

we get the Hamiltonian of the dynamical system

$$H(x, y)=\frac{1}{2}\left(y_r-\frac{e}{mc}A_r\right)\left(y_r-\frac{e}{mc}A_r\right)+\frac{e}{m}A$$

and the differential form

$$\omega_d=y_r\,dx_r-H\,dt.$$

The equation of motion can be put in the form

$$\delta\omega_d-d\omega_\delta=0$$

provided the symbol d defines a displacement along the path, the symbol δ defining an arbitrary displacement.[2)]

If the differential form ω_d be transformed into a perfect differential, the equation of motion will be solved.

Corresponding to 4 types of representation in § 2, we have 4 types of equation of motion.

We denote by (x_r, y_r) canonical variables at $t=t_1$, by (a_r, b_r) canonical variables at $t=t_0$.

1) $$-\frac{\partial U}{\partial t}=H\left(x, \frac{\partial U}{\partial x}\right)=H\left(a, -\frac{\partial U}{\partial a}\right),$$

2) $$-\frac{\partial V}{\partial t}=H\left(x, \frac{\partial V}{\partial x}\right)=H\left(\frac{\partial V}{\partial b}, b\right),$$

3) $$-2\frac{\partial F}{\partial t}=H\left(u-\frac{\partial F}{\partial v}, v+\frac{\partial F}{\partial u}\right)=H\left(u+\frac{\partial F}{\partial v}, v-\frac{\partial F}{\partial u}\right),$$

4) $$-2\frac{\partial G}{\partial t}=H\left(u-\frac{\partial G}{\partial v}, v+\frac{\partial G}{\partial u}\right)=H\left(-u-\frac{\partial G}{\partial v}, -v+\frac{\partial G}{\partial u}\right),$$

$$t=t_1-t_0.$$

§ 4. The coordinate-coordinate transformation

Representing the required contact transformation for a coordinate-coordinate transformation as

$$x_r\,dy_r+b_r\,da_r=dV(y, a),$$

we have

$$x_r=\frac{\partial V}{\partial y_r}=x_r(a),$$

$$V=y_r\,x_r(a)+f(a),$$

$$b_r=y_s\frac{\partial x_s}{\partial a_r}+\frac{\partial f}{\partial a_r}.$$

Since the Hamiltonian is invariant, we have

$$H(x_r(a), y_r) = H\left(a_r, y_s \frac{\partial x_s}{\partial a_r} + \frac{\partial f}{\partial a_r}\right) \tag{2}$$

or, from (1)

$$\frac{1}{2}\left(y_r - \frac{e}{mc} A_r(x)\right)\left(y_r - \frac{e}{mc} A_r(x)\right) + \frac{e}{m} A(x)$$

$$\equiv \frac{1}{2}\left(y_r \frac{\partial x_r}{\partial a_i} + \frac{\partial f}{\partial a_i} - \frac{e}{mc} A_i(a)\right)\left(y_s \frac{\partial x_s}{\partial a_i} + \frac{\partial f}{\partial a_i} - \frac{e}{mc} A_i(a)\right) + \frac{e}{m} A(a). \tag{2'}$$

Equating the coefficients of terms of the same degree in y_r in both members, we get 3 conditions

$$\delta_{rs} = \frac{\partial x_r}{\partial a_i} \frac{\partial x_s}{\partial a_i}, \tag{3}$$

$$A_r(x) = \frac{\partial x_r}{\partial a_i}\left(A_i(x) - \frac{mc}{e} \frac{\partial f}{\partial a_i}\right), \tag{4}$$

$$\frac{1}{2}\left(\frac{e}{mc}\right)^2 A_r(x) A_r(x) + \frac{e}{m} A(x) = \frac{1}{2}\left(\frac{e}{mc} A_i(a) - \frac{\partial f}{\partial a_i}\right)\left(\frac{e}{mc} A_i(a) - \frac{\partial f}{\partial a_i}\right) + \frac{e}{m} A(a). \tag{5}$$

The condition (3) implies that the transformation $a_r \to x_r$ is an orthogonal transformation. Hence we have

$$\frac{\partial x_r}{\partial a_i} \frac{\partial x_r}{\partial a_j} = \delta_{ij}, \tag{3'}$$

and the invariance of the line element

$$dx_r dx_r = da_r da_r,$$

which resembles the property of a perfect instrument in geometrical optics.[3]

Multiplying (4) by $dx_r = (\partial x_r / \partial a_j)\, da_j$ and summing up with respect to r, we have

$$A_r(x)\, dx_r = \frac{\partial x_r}{\partial a_j} \frac{\partial x_r}{\partial a_i}\left(A_i(a) - \frac{mc}{e} \frac{\partial f}{\partial a_i}\right) da_j$$

$$= A_j(a)\, da_j - \frac{mc}{e}\, df \qquad \text{by (3')}. \tag{4'}$$

The function f induces a gauge transformation. Since the gauge transformation does not alter the motion of a particle, f may be dropped from the expressions.

If we eliminate f from (4') by exterior differentiation, we get

$$\left(\frac{\partial A_r}{\partial x_s} - \frac{\partial A_s}{\partial x_r}\right) dx_r \delta x_s = \left(\frac{\partial A_i}{\partial a_k} - \frac{\partial A_k}{\partial a_i}\right) da_i \delta a_k$$

or

$$f_{rs}(x)\, dx_r\, \delta x_s = f_{ik}(a)\, da_i\, \delta a_k, \tag{4''}$$

f_{rs} denoting the magnetic field strength.

The condition (5) is now simplified in a form

$$A(x)=A(a). \tag{5'}$$

§ 5. The momentum-coordinate transformation

In a momentum-coordinate transformation, the final coordinate x_r are functions of the initial momenta b_r alone. Hence b_r are functions of x_r alone. Thence we take a contact transformation

$$y_r dx_r - b_r da_r = dU(x, a)$$

with independent variables x_r, a_r. Since b_r are independent from a_r, we have

$$b_r = -\frac{\partial U}{\partial a_r} = b_r(x)$$

and

$$U = -a_r b_r(x) + f(x),$$

$$y_r = -a_s \frac{\partial b_s}{\partial x_r} + \frac{\partial f}{\partial x_r}.$$

As in the preceding section, f may be dropped. A necessary condition for the momentum-coordinate transformation is then written

$$H\left(x_r, -a_s \frac{\partial b_s}{\partial x_r}\right) = H\left(a_r, b_r(x)\right). \tag{6}$$

If we put

$$H(x, y) = \frac{1}{2} y_r y_r - y_r B_r(x) + B(x),$$

$$B_r(x) = \frac{e}{mc} A_r(x),$$

$$B(x) = \frac{1}{2}\left(\frac{e}{mc}\right)^2 A_r(x) A_r(x) + \frac{e}{m} A(x),$$

the condition (6) will be

$$\frac{1}{2} a_i a_k \frac{\partial b_i}{\partial x_r} \frac{\partial b_k}{\partial x_r} + a_i \frac{\partial b_i}{\partial x_r} B_r(x) + B(x)$$

$$= \frac{1}{2} b_i(x) b_i(x) - b_r(x) B_r(a) + B(a). \tag{6'}$$

The constant terms in $B_r(x)$ and $B(x)$ are indifferent to the motion of a particle. So we can put

$$B_r(0) = B(0) = 0.$$

Putting $a_i=0$ in (6′), we have

$$B(x)=\frac{1}{2}b_i(x)\,b_i(x). \tag{7}$$

Putting $x_i=0$, we see

$$0=\frac{1}{2}b_i(0)\,b_i(0).$$

Consequetly $b_i(x)$ are linearly homogeneous in x_r and $B(x)$ is a quadratic homogeneous form in x_r.

Putting $x_i=0$ in (6′), we have

$$B(a)=\frac{1}{2}a_ia_k\frac{\partial b_i}{\partial x_r}\frac{\partial b_k}{\partial x_r} \tag{8}$$

whence

$$a_i\frac{\partial b_i}{\partial x_r}B_r(x)=-b_r(x)\,B_r(a_r). \tag{9}$$

Hence $B_r(x)$ are linearly homogeneous in x_r. Therefore $H(x,y)$ takes the form

$$H=\frac{1}{2}y_ry_r-\beta_{rs}y_r\,x_s+\frac{1}{2}\gamma_{rs}x_rx_s,$$

$$\beta_{rs}=-\beta_{sr},\quad \gamma_{rs}=\gamma_{sr},\quad B_r(x)=\beta_{rs}x_s,\quad B(x)=\frac{1}{2}\gamma_{rs}x_rx_s.$$

The antisymmetry of β_{rs} is attained by an appropriate gauge transformation.

If we use matrix notations,

$$\|\beta_{rs}\|=\beta,\quad \|\gamma_{rs}\|=\gamma,\quad \|a_{rs}\|=a,\quad \|c_{rs}\|=C$$

where c_{rs} and a_{rs} are defined by

$$b_r(x)=c_{rs}x_s,$$

$$\frac{e}{m}A(x)=\frac{1}{2}a_{rs}x_rx_s,\quad a_{rs}=a_{sr},$$

with an additional condition $\Delta A=0$ or

$$a_{11}+a_{22}+a_{33}=0, \tag{10}$$

the conditions to C (7), (8), (9) turn out to be

$$\gamma=C^*C,\qquad * : \text{transposition} \tag{7′}$$

$$\gamma=CC^*, \tag{8′}$$

$$C\beta=\beta C. \tag{9′}$$

On the other hand, we see

$$\gamma=a+\beta^*\beta=a-\beta^2.$$

So the condition (10) is equivalent to

$$tr\ \gamma = -tr\ \beta^2. \tag{10'}$$

When no magnetic field is present, we have $\beta=0$, $tr\ \gamma=0$. But $tr\ \gamma=tr\ C^*C=c_{ij}c_{ij}$. Hence $C=0$. Therefore the momentum-coordinate transformation is impossible.

In passing we may remark here that the velocity-coordinate transformation is impossible.

Denoting the initial and final velocities by c_r and c'_r, we take the contact transformation

$$\left(v_r+\frac{e}{mc}A_r(x)\right)dx_r-\left(c_r+\frac{e}{mc}A_r(a)\right)da_r=dW(x,\ a).$$

Since x_r depend on only c_r, c_r are functions of x_r alone. Hence we have

$$c_r(x)+\frac{e}{mc}A_r(a)=-\frac{\partial W}{\partial a_r}$$

from which we get the vanishing of magnetic field

$$\frac{\partial A_r}{\partial a_s}-\frac{\partial A_s}{\partial a_r}=0.$$

When the magnetic field is absent, the velocities coincide with the momenta, and the momentum-coordinate transformation is impossible as is seen above. So the velocity-coordinate transformation is impossible.

§ 6. An example of field allowing the two contact transformations

To exhaust all possible types of electromagnetic field in which a specified contact transformation is realizable seems to be a difficult problem. So here will be presented only an example of the electromagnetic field that generates a coordinate-coordinate transformation as well as a momentum-coordinate transformation.

If the constant magnetic field is taken to be parallel to the x_3-axis, the matrix β assumes the form

$$\beta=\begin{Vmatrix} 0 & \omega & 0 \\ -\omega & 0 & 0 \\ 0 & 0 & 0 \end{Vmatrix}.$$

Accordingly the matrix C that commutes with β takes a form

$$C=\begin{Vmatrix} c_{11} & c_{12} & 0 \\ -c_{12} & c_{22} & 0 \\ 0 & 0 & c_{33} \end{Vmatrix}.$$

The conditions (7), (8) require $CC^*=C^*C$, hence

$$(c_{11}-c_{22})c_{12}=0.$$

We pick up the case $c_{11}=c_{22}=\lambda$. Then the matrix γ is written

$$\gamma=\begin{Vmatrix} \lambda^2 & 0 & 0 \\ 0 & \lambda^2 & 0 \\ 0 & 0 & \nu^2 \end{Vmatrix}, \quad \nu=c_{33}.$$

The condition (10′) claims

$$2\lambda^2+\nu^2=2\omega^2. \tag{10''}$$

The Hamiltonian H takes then the form

$$H=\frac{1}{2}(y_1^2+y_2^2+y_3^2)-\omega(y_1x_2-y_2x_1)+\frac{1}{2}(\lambda^2x_1^2+\lambda^2x_2^2+\nu^2x_3^2).$$

We perform the change of variables $(x_i, y_i)\to(\xi_i, \eta_i)$ by a contact transformation with its generating function $S(x, \eta, t)$,

$$S=\eta_1(x_1\cos\omega t+x_2\sin\omega t)+\eta_2(-x_1\sin\omega t+x_2\cos\omega t)+\eta_3x_3,$$

$$dS=y_i\,dx_i+\xi_i\,d\eta_i+(\partial S/\partial t)\,dt.$$

We have then

$$\xi_1=x_1\cos\omega t+x_2\sin\omega t, \quad \xi_2=-x_1\sin\omega t+x_2\cos\omega t, \quad \xi_3=x_3,$$

$$\eta_1=y_1\cos\omega t+y_2\sin\omega t, \quad \eta_2=-y_1\sin\omega t+y_2\cos\omega t, \quad \eta_3=y_3,$$

$$\frac{\partial S}{\partial t}=\omega(\eta_1\xi_2-\eta_2\xi_1).$$

The contact transformation brings the linear form $\omega_a=y_i\,dx_i-H\,dt$ into

$$dS-\xi_i\,d\eta_i-\frac{\partial S}{\partial t}dt-Hdt=d(S-\xi_i\eta)+\eta_i d\xi_i-\left(H+\frac{\partial S}{\partial t}\right)dt.$$

Hence the Hamiltonian for the transformed system turns out to be

$$H+\frac{\partial S}{\partial t}=\frac{1}{2}(\eta_1^2+\eta_2^2+\eta_3^2)+\frac{1}{2}(\lambda^2\xi_1^2+\lambda^2\xi_2^2+\nu^2\xi_3^2).$$

The preceding transformation represents the transition from the old coordinate system to a coordinate system rotating with the angular velocity ω around the x_3-axis.

The motion of a particle observed in the rotating coordinate system is the superposition of simple harmonic motions in 3 mutually orthogonal directions.

Two cases are distinguished:

1) $\lambda=\nu$. From (10″) we have

$$\lambda^2=\nu^2=2\omega^2/3.$$

The dynamical system with its Hamiltonian

$$H=\frac{1}{2}(\eta_1^2+\eta_2^2+\eta_3^2)+\frac{\nu^2}{2}(\xi_1^2+\xi_2^2+\xi_3^2)$$

generates clearly a coordinate-coordinate transformation as well as a momentum-coordinate transformation, and transition to the old coordinate system does not alter the character of the 2 contact transformations.

The field selected above is represented by

$$f_{23}=f_{31}=0, \quad \frac{e}{mc} f_{12}=2\omega=\sqrt{6}\,\nu ,$$

$$\frac{e}{m}A(x)=\frac{\nu^2}{4}(-x_1^2-x_2^2+2x_3^2).$$

The motion of a particle, however, is not periodic if observed in the old (or fixed) coordinate system, since $\omega/\nu=(3/2)^{1/2}$ is not a rational number.

2) purely periodic motion. In this case λ, ν, ω must be commensurable. The homogeneous Diophantine equation

$$2\lambda^2+\nu^2=2\omega^2$$

has an infinite number of integral solutions with no common divisor, e.g.

$$(\lambda:\nu:\omega)=(1:4:3),\ (7:8:9),\ (7:12:11),\ (17:12:19),\ \text{etc.}$$

Fields corresponding to each of the solutions are

$$f_{23}=f_{31}=0, \quad \frac{e}{mc} f_{12}=2\omega,$$

$$\frac{e}{m}A(x)=\frac{\nu^2}{4}(-x_1^2-x_2^2+2x_3^2),$$

$$\frac{\omega}{\nu}=\frac{3}{4},\ \frac{9}{8},\ \frac{11}{12},\ \frac{19}{12},\ \text{etc.}$$

Dynamical systems in this case perform only the coordinate-coordinate transformation.

References

1) H. Weyl, *Classical Groups* (Princeton University Press 1946), 169.
2) E. Cartan, *Leçons ur les invariants nitegraux* (Hermann, Paris 1922), 17–19.
3) C. Caratheodory, *Geometrische Optik* (Springer. Berlin 1937), 72–77.

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On the Self-stress

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The reason why the difficulty pointed out by Pais arises is analized by the general discussion independent of any approximation for the self-stress of an arbitrary elementary particle interacting with arbitrary fields. To do this, the Pais-Epstein-Sawada's formula is generalized for the system with more intricate interaction. The difficulty due to the process of the vacuum polarization type on account of which the non-vanishing self-stress has been given is also discussed.

§ 1. Introduction

In 1949 Pais proposed the following important problem :[1] In the relativistic field theory, the energy-momentum tensor $T_{\mu\nu}$ of the system of the particle and field must satisfy the transformation relation

$$E(v)=\frac{E(0)-v^2S(0)}{\sqrt{1-v^2}}\text{ *)},\qquad (1\cdot1)$$

where $E=\int T_{44}dv$ and $S=\int T_{11}dv$ and the arguments 0 and v of E and S mean the velocities of the electron. Equation $(1\cdot1)$ holds true in classical theory as well as in quantum theory, provided that in the latter case we consider the energy and the stress as the expectation values referring to the specified states of the system. From $(1\cdot1)$, we can easily see that if the energy E has the transformation property of the inertia mass, the stress $S(0)$ must be zero in all cases. One finds, however, that up to the second order in e,

$$S(0)=-\frac{e^2}{2\pi}\mu\qquad (1\cdot2)$$

with the mass μ of the electron. On the other hand, we should expect that the self-energy directly calculated by the covariant procedure[2] or by the w-method[3] has the transformation property of the inertia mass. This fact is definitely inconsistent with $(1\cdot2)$.

J. Yukawa and one of the authors (H.U.)[4] have clarified the cause of the above contradiction. According to their theory, this contradiction arises from the introduction of the radius as the cut off factor of the diverging self-energy in conflict with the point model of the electron in the theory of the quantum fields ; namely, the self-energy of the

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* We adopt the natural unit throughout this paper, i.e., $\hbar=c=1$.

electron due to the electromagnetic field in the second order in e

$$\delta\mu=\frac{3e^2}{2\pi}\mu\left(\log\frac{K+\sqrt{K^2+\mu^2}}{\mu}-\frac{1}{6}\right)$$

is proportional to μ if only we put $b\equiv\frac{1}{K}$ and approach b to zero (the radius of the electron tends to zero). Therefore

$$S(0)=\frac{1}{3}\left(\mu\frac{\partial\delta\mu}{\partial\mu}-\delta\mu\right)=0.$$

In our paper we shall prove that *the above conclusion holds true in the case when an arbitrary elementary particle is interacting with an arbitrary field via more intricate couplings in any order of the perturbation approximation.*

In order to proceed with our discussion in a concrete form as much as possible, in section 2 we begin with the discussions of the systems of the electron interacting with the electromagnetic field via the vector and the tensor coupling separately. Section 3 deals with the consideration of the electron interacting with the charged and neutral scalar meson field via the scalar and vector couplings. Section 4 is devoted to discuss generally the self-stress of an arbitrary elementary particle due to an arbitrary field. In APPENDIX 2, the process of the vacuum polarization type which gives the non-vanishing self-stress will be discussed.

Recently the applicability of the renormalization theory has been discussed by Sakata, Umezawa and Kamefuchi[5] and it has been clarified that the system with the "interaction of the second kind" requires the infinite number of the counter terms. Since the infinite number of the counter terms are required means that elementary particle has the finite extention, it becomes an important problem that we examine in the frame of the present theory whether or not the elementary particle will also behave as a particle in the inre-normalizable region. It will be seen in our paper that the self-stress also vanishes in such a system.

We shall briefly write the synopsis of our discussion in the following:

1) The energy-momentum tensor[6] is defined from the Lagrangian L by

$$T_{\mu\nu}=\frac{\partial L}{\partial\frac{\partial\varphi_\alpha}{\partial x_\mu}}\frac{\partial\varphi_\alpha}{\partial x_\nu}-\delta_{\mu\nu}L. \tag{1·3}$$

2) The expectation value of the trace of the energy-momentum tensor for the one particle at rest becomes the form

$$\left\langle\int T_{\mu\mu}dv\right\rangle=\left(\mu\frac{\partial\delta\mu}{\partial\mu}+\varkappa\frac{\partial\delta\mu}{\partial\varkappa}-g\frac{\partial\delta\mu}{\partial g}+\mu\right), \tag{1·4}$$

where $\int dv$ stands for the spatial integration and μ, $\varkappa$ and g mean the masses of the source and the field and the coupling constant of the derivative interaction respectively.

3) In the system we concern, the quantities with the dimension of the length which can contribute to the self-energy are

$$[\mu]=[\varkappa]=L^{-1} \quad \text{and} \quad [g]=L,$$

so we cannot help making the self-energy

$$\delta\mu=\sum a_{ij}^{n} g^{n} \mu^{i} \varkappa^{j} \tag{1·5}$$

under the condition $i+j-n=1$ and with the dimensionless constants a_{ij}^{n}. Therefore one easily obtains, substituting (1·5) in (1·4),

$$\langle \int T_{\mu\mu} dv \rangle = \delta\mu+\mu. \tag{1·6}$$

4) We have, for symmetry reasons[1],

$$S(0)=\frac{1}{3}\{\langle \int T_{\mu\mu} dv \rangle - E(0)\} \tag{1·7}$$

$$=\frac{1}{3}\{\delta\mu+\mu-\delta\mu-\mu\}=0. \tag{1·8}$$

Now, let us notice the following fact: in the perturbation calculation, as a result of the diverging self-energy we must temporarily cut off in course of the calculation[4]. If we denote this inevitable cut off radius of the elementary particle by b, the form

$$\delta\mu=\sum a_{ij}^{n\alpha} g^{n} \mu^{i} \varkappa^{j} b^{\alpha} \text{ *)}$$

with $i+j-\alpha-n=1$ and $\alpha \neq 0$ is permitted. From (1·4) and (1·7), we obtain

$$S(0)=\frac{1}{3}\sum \alpha\, a_{ij}^{n\alpha} g^{n} \mu^{i} \varkappa^{j} b^{\alpha}. \tag{1·9}$$

Even if this series were vanishing, b would become the function of μ and $\varkappa$ and this fact is inconsistent with the assumption referring to the derivation of (1·4) that is obtained by the integration with the limits independent of the mass**). Therefore it never happen that the series (1·9), viz. the self-stress vanishes. The validity of the foregoing procedure by Yukawa and one of us (H.U.)[4] in the second order of the perturbation calculation has been confirmed by the general dimensional consideration.

§ 2. The self-stress of the electron due to the electromagnetic field

The electron interacting with the electromagnetic field via the vector coupling is characterized by the Lagrangian

$$L=-\bar{\psi}\left(\gamma_{\mu}\frac{\partial}{\partial x_{\mu}}+\mu\right)\psi+ie\,\bar{\psi}\gamma_{\mu}\psi A_{\mu}-\frac{1}{2}\frac{\partial A_{\mu}}{\partial x_{\nu}}\frac{\partial A_{\mu}}{\partial x_{\nu}}. \tag{2·1}$$

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* If it is impossible to expand to the series, we may adopt the forms $\delta\mu=\mu f(\mu/\varkappa, g\mu)$ and $\delta\mu=\mu f(\mu/\varkappa, g\mu, a\mu)$ respectively, so we shall obtain the same conclusion as easily seen.

** Note added in proof: In this meaning, the discussion of S. Borowitz and W. Kohn in the appendix 1 of the Physical Review **86**, (1952), 985 is incorrect, which we have seen recently.

According to (1·1), we obtain

$$T_{\mu\mu}=\mu\bar{\psi}\psi+ie\,\bar{\psi}\gamma_\mu\psi A_\mu+\frac{\partial A_\mu}{\partial x_\nu}\frac{\partial A_\mu}{\partial x_\nu}. \tag{2·2}$$

This is settled not only in Heisenberg representation, but also in interaction representation. Now we will calculate the expectation value of (2·2) for the state in which there is one electron at rest in the remote past and infinite future, namely it turns out to adopt the mixed representation of Dyson, so we may integrate it over all four-dimensional space and omit finally the time integral, because to do so becomes to pick up the part of the matrix element in which the energy is conserved.

Throughout our calculation, we will disregard the normal-dependent terms which as shown by Koba[7], disappear at last*). If we put

$$A\equiv\frac{\partial A_\mu}{\partial x_\nu}\frac{\partial A_\mu}{\partial x_\nu}, \tag{2·3}$$

$$H\equiv-ie\,\bar{\psi}\gamma_\mu\psi A_\mu, \tag{2·4}$$

the expectation value of A for the one electron state is

$$\left\langle\int A dx\right\rangle=\left\langle\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int dx\int dx_1\ldots\int dx_n P(\boldsymbol{A}(x),\ \boldsymbol{H}(x_1),\ldots,\ \boldsymbol{H}(x_n))\right\rangle^{**}. \tag{2·5}$$

Let us consider about a certain term in right hand side of (2·5), so this is that $\boldsymbol{A}(x)$ enters into one of the photon lines in the self-energy graph***), and this means that the term

$$2\int\frac{1}{2}\frac{\partial D_F(x'-x)}{\partial x_\lambda}\frac{1}{2}\frac{\partial D_F(x-x'')}{\partial x_\lambda}dx$$

is substituted instead of the internal photon line

$$\frac{1}{2}D_F(x'-x'').$$

Integrating partially and usidg (A·1), we have

$$2\int\frac{1}{2}\frac{\partial D_F(x'-x)}{\partial x_\lambda}\frac{1}{2}\frac{\partial D_F(x-x'')}{\partial x_\lambda}dx=-2i\frac{1}{2}D_F(x'-x'').$$

$\boldsymbol{A}(x)$ has the $n/2$ positions to insert in the self-energy graph of the n-th order in the perturbation calculation, so

* Discussion by Koba in the S-matrix form can be developed for the case of the physical quantities in Heisenberg representation. We will discuss this point in detail in our forthcoming paper.

** Throughout this paper, the bold letter means the quantities in interaction representation and $\langle\ \rangle$ expresses the expectation value refering to the state in which one particle rests.

*** See Appendix (II) about the "self-energy graph".

$$\left\langle \int A(x)dx \right\rangle = -\left\langle \sum_{n=0}^{\infty} \int n\,\delta\mu^{(n)}\bar{\psi}\psi\,dx \right\rangle$$

$$= -\left\langle e\frac{\partial \delta\mu}{\partial e}\int \bar{\psi}\psi\,dx \right\rangle, \qquad (2\cdot6)$$

where $\delta\mu^{(n)}$ means the n-th order term of the self-energy in the perturbation calculation. In similar manner, we have

$$\left\langle \int H(x)dx \right\rangle = -e\frac{\partial \delta\mu}{\partial e}\left\langle \int \bar{\psi}\psi\,dx \right\rangle. \qquad (2\cdot7)$$

In the next, operate $\mu\dfrac{\partial}{\partial\mu}$ on the matrix element corresponding to a certain self-energy graph, so one of the internal electron lines

$$\frac{1}{2}S_F(x'-x'')$$

becomes, by (A·5),

$$i\int \frac{1}{2}S_F(x'-x)\frac{1}{2}S_F(x-x'')\,dx,$$

or the external electron line $\psi(x)$ is changed into

$$i\int \frac{1}{2}S_F(x-x')\psi(x')\,dx'.$$

Ultimately, we have

$$\mu\frac{\partial \delta\mu}{\partial\mu}\left\langle \int \bar{\psi}\psi dx \right\rangle = \mu\left\langle \int \bar{\psi}\psi\,dx \right\rangle - i\delta\mu\left\langle \int \bar{\psi}(x)\,S_F(x-x')\psi(x')\,dx dx' \right\rangle^{*)}.$$

The second term in the right hand side of this equation diverges, for $\psi(x)$ and $S_F(x-x')$, respectively, obey homogeneous and inhomogeneous equations associated with the same differential operator. Physically speaking, this term stands for the effect, in Dyson formalism, that the electron emits and absorbs the photons for a long time before the scattering. Therefore we can eliminate this term by the renormalization (for instance, the renormalization may be performed by the method of Kamefuchi-Umezawa; Prog. Theor. Phys. 7 (1952), 399). We obtain, just then,

$$\mu\left\langle \int \bar{\psi}\psi dx \right\rangle = \mu\frac{\partial \delta\mu}{\partial\mu}\left\langle \int \bar{\psi}\psi\,dx \right\rangle. \qquad (2\cdot8)$$

From (2·6), (2·7) and (2·8), it is easily seen that

$$\left\langle \int T_{\mu\mu}dv \right\rangle = \mu\frac{\partial \delta\mu}{\partial\mu} + \mu, \qquad (2\cdot9)$$

---

* See Appendix (II).

in all order of the perturbation calculation. As $\delta\mu$ is to be proportional to μ in this system from the dimensional consideration, we observe that the self-stress vanishes according to the consideration at the end of section 1.

We shall now treat the system that the electron is interacting with the electromagnetic field *via the Pauli-type coupling.*[5] We have the Lagrangian of this system

$$L=-\bar{\psi}\left(\gamma_\mu\frac{\partial}{\partial x_\mu}+\mu\right)\psi+\varepsilon\bar{\psi}O^{\mu\nu}\psi\frac{\partial A_\mu}{\partial x_\nu}-\frac{1}{2}\frac{\partial A_\mu}{\partial x_\nu}\frac{\partial A_\mu}{\partial x_\nu}. \tag{2·10}$$

When we manage similarly for

$$T_{\mu\mu}=\mu\bar{\psi}\psi+\frac{\partial A_\mu}{\partial x_\nu}\frac{\partial A_\mu}{\partial x_\nu}, \tag{2·11}$$

it is found that

$$\left\langle\int T_{\mu\mu}\,dv\right\rangle=\mu\frac{\partial\delta\mu}{\partial\mu}-\varepsilon\frac{\partial\delta\mu}{\partial\varepsilon}+\mu. \tag{2·12}$$

So long as this system is concerned, we have two quantities with the dimension of length

$$[\mu]=L^{-1} \qquad \text{and} \qquad [\varepsilon]=L,$$

hence we can put

$$\delta\mu=\sum a_n\,\varepsilon^n\,\mu^{n+1}.$$

Therefore the self-stress also vanishes from (1·6).

§ 3. The self-stress of the electron due to the scalar meson field

There was the special situation in the previous section that the field interacting with the electron is of zero-mass and neutral. But this section is devoted to confirm the same conclusion as the previous section for the neutral and the charged scalar mesons with the finite mass $\varkappa$ interacting with the electron. The Lagrangian is

$$L=-\bar{\psi}\left(\gamma_\mu\frac{\partial}{\partial x_\mu}+\mu\right)\psi-\frac{1}{2}\left(\frac{\partial\phi^\alpha}{\partial x_\nu}\frac{\partial\phi^\alpha}{\partial x_\nu}+\varkappa^2\phi^\alpha\phi^\alpha\right)$$

$$+f^\alpha\bar{\psi}O^\alpha\psi\phi^\alpha+g^\alpha\bar{\psi}O^\alpha_\mu\psi\frac{\partial\phi^\alpha}{\partial x_\mu}\ ^{*)}, \tag{3·1}$$

where α is the suffix in the isotopic spin space. In conformity to the same manner as in the section 1, we have

$$T_{\mu\mu}=\mu\,\bar{\psi}\,\psi+\varkappa^2\phi^\alpha\,\phi^\alpha-f^\alpha\bar{\psi}O^\alpha\psi\,\phi^\alpha+\Phi, \tag{3·2}$$

with

$$\Phi=\frac{\partial\phi^\alpha}{\partial x_\lambda}\frac{\partial\phi^\alpha}{\partial x_\lambda}+\varkappa^2\phi^\alpha\phi^\alpha. \tag{3·3}$$

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* The gradient coupling term is meaningful for the charged meson rather than the neutral one.

We will evaluate the correction of (3·3) by the interaction

$$\boldsymbol{H}=-f^{\alpha}\bar{\boldsymbol{\phi}}O^{\alpha}\boldsymbol{\phi}\boldsymbol{\phi}^{\alpha}-g^{\alpha}\bar{\boldsymbol{\phi}}O_{\mu}^{\alpha}\boldsymbol{\phi}\frac{\partial\boldsymbol{\phi}^{\alpha}}{\partial x_{\mu}}+\text{normal dependent term.} \tag{3·4}$$

We may again talk about this correction by integrating over whole 4-space to omit finally the time integral in same reason as in the foregoing section, so

$$\left\langle\int \Phi dx\right\rangle=-\left\langle f^{\alpha}\frac{\partial\delta\mu}{\partial f^{\alpha}}\int\bar{\boldsymbol{\phi}}\boldsymbol{\phi}\,dx\right\rangle-\left\langle g^{\alpha}\frac{\partial\delta\mu}{\partial g^{\alpha}}\int\bar{\boldsymbol{\phi}}\boldsymbol{\phi}\,dx\right\rangle, \tag{3·5}$$

$$\left\langle\int f^{\alpha}\bar{\psi}O^{\alpha}\psi\,\phi^{\alpha}dx\right\rangle=-\left\langle f^{\alpha}\frac{\partial\delta\mu}{\partial f^{\alpha}}\int\bar{\boldsymbol{\phi}}\boldsymbol{\phi}\,dx\right\rangle. \tag{3·6}$$

By means of (A·4) and (A·5), we have

$$\left\langle\varkappa^{2}\int\phi^{\alpha}\phi^{\alpha}dx\right\rangle=\left\langle\varkappa\frac{\partial\delta\mu}{\partial\varkappa}\int\boldsymbol{\phi}^{\alpha}\boldsymbol{\phi}^{\alpha}dx\right\rangle \tag{3·7}$$

and

$$\left\langle\mu\int\bar{\psi}\psi dx\right\rangle=\left\langle\mu\frac{\partial\delta\mu}{\partial\mu}\int\bar{\boldsymbol{\phi}}\boldsymbol{\phi}\,dx\right\rangle. \tag{3·8}$$

Eventually, from (3·5), (3·6), (3·7) and (3·8), we obtain independently of any approximation,

$$\left\langle\int T_{\mu\mu}dv\right\rangle=\mu\frac{\partial\delta\mu}{\partial\mu}+\varkappa\frac{\partial\delta\mu}{\partial\varkappa}-g^{\alpha}\frac{\partial\delta\mu}{\partial g^{\alpha}}+\mu.$$

The second term of the right hand side of this equation has been obtained by Sawada[8] in the second order of the perturbation calculation. Since we must use the following form of the self-energy

$$\delta\mu=\sum a_{ij}^{\alpha n}(g^{\alpha})^{n}\mu^{i}\varkappa^{j},\quad i+j-n=1,$$

the self-stress also vanishes definitely.

§ 4. The general discussion of the self-stress

The discussion same as in the previous sections comes into existence for most general system. We temporarily restrict ourselves to consider the spinor field ψ, interacting with other boson field Q_{α}. If we denote the total Lagrangian, the free spinor part, the free boson part and interaction part by L, $\mathcal{L}^{\bar{}}$, $\mathcal{L}$ and $\mathcal{L}'$ respectively, these are given as follows:

$$L=\mathcal{L}^{\bar{}}+\mathcal{L}+\mathcal{L}', \tag{4·1}$$

$$\mathcal{L}^{\bar{}}=-\{\bar{\psi}_{i}\chi_{ij}^{\mu}\psi_{j\mu}+\mu\bar{\psi}_{i}\Gamma_{ij}\psi_{j}\}, \tag{4·2}$$

$$\mathcal{L}=-\frac{1}{2}\{X_{\alpha\beta}^{\mu\nu}Q_{\beta\nu}Q_{\alpha\mu}+\varkappa^{2}Y_{\alpha\beta}Q_{\beta}Q_{\alpha}\} \tag{4·3}$$

and

$$\mathcal{L}' = f\bar{\psi}_i O^{\alpha}_{ij}\psi_j Q_\alpha + g\bar{\psi}_i O^{\alpha\mu}_{ij}\psi_j Q_{\alpha\mu}, \tag{4·4}$$

where χ, Γ, X, Y and O are the constants which do not include the field quantities and the both masses and the subscripts μ and ν stand for the derivatives with respect to x_μ and x_ν respectively.

We have, then, the equations of motion

$$\chi^{\mu}_{ij}\psi_{j\mu} + \mu\Gamma_{ij}\psi_j = fO^{\alpha}_{ij}\psi_j Q_\alpha + gO^{\alpha\mu}_{ij}\psi_j Q_{\alpha\mu} \tag{4·5}$$

and

$$X^{\mu\nu}_{\alpha\beta}Q_{\beta\nu\mu} - \varkappa^2 Y_{\alpha\beta}Q_\beta = f\bar{\psi}_i O^{\alpha}_{ij}\psi_j - g(\bar{\psi}_i O^{\alpha\mu}_{ij}\psi_j)_\mu . \tag{4·6}$$

Further,

$$T_{\mu\mu} = \mu\bar{\psi}_i\Gamma_{ij}\psi_j + \varkappa^2 Y_{\alpha\beta}Q_\beta Q_\alpha - f\bar{\psi}_i O^{\alpha}_{ij}\psi_j Q_\alpha + Q, \tag{4·7}$$

with

$$Q = X^{\mu\nu}_{\alpha\beta}Q_{\beta\nu}Q_{\alpha\mu} + \varkappa^2 Y_{\alpha\beta}Q_\beta Q_\alpha . \tag{4·8}$$

We will develop the calculation of the expectation value of one particle of (4·7) to know the relation to the self-energy. As we noted in the section 2, we may talk about the matrix element integrated over the whole four dimensional space to omit finally the time integral, because the energy is conserved between the states of the infinite future and the remote past. As is well-known, the vacuum expectation values $\langle P(\psi_i(x), \psi_j(x'))\rangle_0$ and $\langle P(Q_\alpha(x), Q_\beta(x'))\rangle_0$ are the kernels of respective field, so

$$S_{Fij}(x-x') = 2\langle P(\psi_i(x), \bar{\psi}_j(x'))\rangle_0 = \frac{i}{X^{\mu}_{ij}\partial_\mu + \mu\Gamma_{ij}}\delta(x-x') \tag{4·9}$$

and

$$\Delta_{F\alpha\beta}(x-x') = 2\langle P(Q_\alpha(x), Q_\beta(x'))\rangle_0 = \frac{i}{X^{\mu\nu}_{\alpha\beta}\partial_\mu\partial_\nu - \varkappa^2 Y_{\alpha\beta}}\delta(x-x') \tag{4·10}$$

with the exception of the normal dependent terms*). Therefore, we have the relations

$$\mu\frac{\partial}{\partial\mu}S_{Fij}(x-x') = -i\mu\int S_{Fik}(x-x'')\Gamma_{kl}S_{Flj}(x''-x')\,dx'' \tag{4·11}$$

and

$$\varkappa\frac{\partial}{\partial\varkappa}\Delta_{F\alpha\beta}(x-x') = 2i\varkappa^2\int \Delta_{F\alpha\gamma}(x-x'')Y_{\gamma\delta}\Delta_{F\delta\beta}(x''-x')\,dx''. \tag{4·12}$$

From (4·11), we can see easily that the operation $\mu\dfrac{\partial}{\partial\mu}$ on one of the internal fermion lines corresponds to insert $\mu\int\bar{\psi}_i\Gamma_{ij}\psi_j dx$ in it as well as $\varkappa\dfrac{\partial}{\partial\varkappa}$ on boson line to $\varkappa^2\int Y_{\alpha\beta}Q_\beta Q_\alpha dx$.

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* (4·9) and (4·10) will be proved in our forthcoming paper.

From

$$(\chi^{\mu}_{ij}\partial_{\mu}+\mu\Gamma_{ij})\psi_j(x)=0$$

and (4·13)

$$(X^{\mu\nu}_{\alpha\beta}\partial_{\mu}\partial_{\nu}-\varkappa^2 Y_{\alpha\beta})\,Q_{\beta}(x)=0,$$

it is obtained for the external line that

$$\mu\frac{\partial}{\partial\mu}\psi_i(x)=-i\mu\int S_{Fij}(x-x')\,\Gamma_{jk}\psi_k(x')\,dx' \tag{4·14}$$

and

$$\left.\begin{aligned}\varkappa\frac{\partial}{\partial\varkappa}Q_{\alpha}(x)&=2i\varkappa^2\int \Delta_{F\alpha\beta}(x-x')\,Y_{\beta\tau}Q_{\tau}(x')\,dx'\\&=2i\varkappa^2\int Q_{\tau}(x')\,Y_{\tau\beta}\Delta_{F\beta\alpha}(x'-x)\,dx'.\end{aligned}\right\} \tag{4·15}$$

Thus we are led to:

$$\begin{aligned}&\langle\mu\int\bar{\psi}_i\Gamma_{ij}\psi_j dx\rangle+\langle\varkappa^2\int Y_{\alpha\beta}Q_{\beta}Q_{\alpha}dx\rangle\\&=\Big(\mu\frac{\partial\delta\mu}{\partial\mu}+\varkappa\frac{\partial\delta\mu}{\partial\varkappa}+\mu\Big)\Big\langle\int\bar{\psi}_i\psi_i dx\Big\rangle \qquad \text{for one fermion state,}\\&=\Big(\mu\frac{\partial\delta\varkappa}{\partial\mu}+\varkappa\frac{\partial\delta\varkappa}{\partial\varkappa}+\varkappa\Big)\Big\langle\int Q_{\alpha}Q_{\alpha}dx\Big\rangle \qquad \text{for one boson state.}\end{aligned} \tag{4·16}$$

Here $\delta\mu$ is the self-energy of the fermion due to the boson and $\delta\varkappa$ the boson's due to the fermion*). Another part of $T_{\mu\mu}$ is, similarly as in the sections 2 and 3,

$$\begin{aligned}&\Big\langle -f\int\bar{\psi}_i O^{\alpha}_{ij}\psi_j Q_{\alpha}dx\Big\rangle+\Big\langle\int Q dx\Big\rangle\\&=\Big\langle -g\frac{\partial\delta\mu}{\partial g}\int\bar{\psi}_i\psi_i dx\Big\rangle, \qquad \text{for fermion,}\\&=\Big\langle -g\frac{\partial\delta\varkappa}{\partial g}\int Q_{\alpha}Q_{\alpha}dx\Big\rangle, \qquad \text{for boson.}\end{aligned} \tag{4·17}$$

One then obtain (1·2), namely,

$$\Big\langle\int T_{\mu\mu}dv\Big\rangle=\begin{cases}\Big(\mu\dfrac{\partial}{\partial\mu}+\varkappa\dfrac{\partial}{\partial\varkappa}-g\dfrac{\partial}{\partial g}\Big)\delta\mu+\mu & \text{for fermion,}\\ \Big(\mu\dfrac{\partial}{\partial\mu}+\varkappa\dfrac{\partial}{\partial\varkappa}-g\dfrac{\partial}{\partial g}\Big)\delta\varkappa+\varkappa & \text{for boson.}\end{cases} \tag{4·18}$$

Using $[\mu]=[\varkappa]=L^{-1}$ and $[g]=L$, we cannot help making the self-energy

$$\left.\begin{matrix}\delta\mu\\ \delta\varkappa\end{matrix}\right\}=\sum a^n_{ij}\,g^n\,\mu^i\,\varkappa^j,\quad i+j-n=1,$$

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* About the self-stress of the photon, see J. Yukawa, H. Umezawa, Prog. Theor. Phys. 6 (1951), 197.

so

$$S(0)=\frac{1}{3}\left\{\left\langle\int T_{\mu\mu}dv\right\rangle-E(0)\right\}=0.$$

The same conclusion is arranged for the boson-boson and the fermion-fermion systems. That the non-vanishing self-stress is obtained by the "cut off" is also the case (cf. (1·9)). Furthermore if we adopt the interaction like $h\bar{\psi}O\psi Q^{\eta}$, we easily obtain

$$\left\langle\int T_{\mu\mu}\,dv\right\rangle=\left\{\mu\frac{\partial}{\partial\mu}+\varkappa\frac{\partial}{\partial\varkappa}-(\eta-1)h\frac{\partial}{\partial h}\right\}\delta\mu+\mu$$

and

$$\delta\mu=\sum a^{n}_{ij}\,h^{n}\mu^{i}\varkappa^{j}$$

with $i+j+n(1-\eta)=1$, so the self-stress also vanishes.

§ 5. Conclusion

We could start from the most general Lagrangian (4·1) to be sure that the self-stress of an arbitrary elementary particle interacting with an arbitrary field also vanishes in any order of the perturbation calculation. In order to do so, we derived the *generalized Pais' formula*

$$\left\langle\int T_{\mu\mu}\,dv\right\rangle=\mu\frac{\partial\delta\mu}{\partial\mu}+\varkappa\frac{\partial\delta\mu}{\partial\varkappa}-g\frac{\partial\delta\mu}{\partial g}+\mu, \qquad (5\cdot1)$$

which holds true in an arbitrary order of the perturbation calculation, and adopted the self-energy $\delta\mu$ in all possible forms which can be obtained from the quantities with the dimension of the mass referring to this system. Originally the quantities which can explicitely contribute to the self-energy are no more than μ, $\varkappa$ and g, so it seems natural that the form (1·5) of the self-energy given at the end of the introduction should be permitted. Unfortunately, however, the "divergence" inherent in the present formalism shades off the conclusion in the dimension analysis based on μ, $\varkappa$ and g, because the temporary entering of the high momentum K in the theory as a cut off factor is necessarily required. The very point gives the non-vanishing self-stress as shown by the dimensional consideration in the introduction. If we understand above fact from the reverse side, the present theory contains *through the "divergence"* not only the quantities explicitely included in the Lagrangian but also the quantities with the dimension of the length such as the cut off radius and so this factor (on account of the divergence) gave the non-vanishing self-stress. Thus *the difficulty pointed out by Pais is not the primary proper problem by itself and may be transformed into the problem of the self-energy by way of the generalized Pais' formula* (5·1). Anyhow, it may be said that the present quantum theory which is formally covariant cannot avoid the unsatisfactory point on the view of the relativity only because of the "divergence".

We thank Prof. S. Sakata for his continual encouragement and Mr. S. Kamefuchi ofr his valuable discussion and pertinent criticism.

Appendix

(I) On the operators $\mu\frac{\partial}{\partial\mu}$ and $x\frac{\partial}{\partial x}$

$$(\Box-\varkappa^2)\,\Delta_F(x-x')=2i\delta(x-x'). \tag{A·1}$$

$$\left(\gamma_\mu\frac{\partial}{\partial x_\mu}+\mu\right)S_F(x-x')=2i\,\delta(x-x'). \tag{A·2}$$

If we operate $x\frac{\partial}{\partial x}$ on both sides of (A·1), we have

$$(\Box-\varkappa^2)\,x\frac{\partial}{\partial x}\Delta_F(x-x')=2\varkappa^2\Delta_F(x-x'). \tag{A·3}$$

By deviding both sides by $\Box-\varkappa^2+i\varepsilon$, we obtain

$$x\frac{\partial}{\partial x}\Delta_F(x-x')=-i\int\Delta_F(x-x'')\,\Delta_F(x''-x')\,dx''. \tag{A·4}$$

Similarly for S_F, we obtain

$$\mu\frac{\partial}{\partial\mu}S_F(x-x')=\frac{i}{2}\int S_F(x-x'')\,S_F(x''-x')\,dx''. \tag{A·5}$$

For the external electron line,

$$\left(\gamma_\mu\frac{\partial}{\partial x_\mu}+\mu\right)\phi(x)=0.$$

Therefore

$$\mu\frac{\partial}{\partial\mu}\phi(x)=\frac{i}{2}\int S_F(x-x'')\,dx''\phi(x''). \tag{A·6}$$

(II) On the processes of the type of the "vacuum polarization"

The correction of $\bar{\psi}\psi$ involving the *essential part* which is connected to the other electron line by a single boson line with zero momentum is just what is usually called the correction of the "*vacuum polarization type*" (see Fig. 1). Such the correction of $\bar{\psi}\psi$ has had, under certain circumstances, the contribution which is not obtained by differentiating with respective to μ the *ordinary* self-energy $\delta\mu$ in which the correction like Fig. 3 is included. However if we adopt the self-energy $\delta\mu$ containing the processes such as Fig. 2, $\mu\frac{\partial\delta\mu}{\partial\mu}$ is just the total one-particle-correction of $\mu\int\bar{\psi}\psi dv$. If we transform the Schrödinger equation

$$i\frac{\delta\Psi(\sigma)}{\delta\sigma(x)}=H(x)\Psi(\sigma)$$

with

$$H(x)=-f\bar{\psi}O_\alpha\psi Q_\alpha \tag{A·7}$$

by

$$\Psi(\sigma)\to S(\sigma)\Psi(\sigma),$$

$$S(\sigma)=\exp\left\{-i\int_{-\infty}^{\sigma}H(x')dx'\right\}, \tag{A·8}$$

the new state vector satisfies the equation

$$i\frac{\delta\Psi(\sigma)}{\delta\sigma(x)}=\left[-\frac{f^2}{4}\int\{\rho_\alpha(x),\ \rho_\beta(x')\}\bar{\Delta}_{\alpha\beta}(x-x')dx'\right.$$
$$\left.-\frac{if^2}{8}\int[\rho_\alpha(x),\ \rho_\beta(x')]\{Q_\alpha(x),\ Q_\beta(x')\}\varepsilon(x-x')dx'\right]\Psi(\sigma), \tag{A·9}$$

to the required order of approximation, where

$$\rho_\alpha(x)\equiv\bar{\psi}(x)O_\alpha\psi(x).$$

It is needless to say that the one particle component of

$$\{\rho_\alpha(x),\ \rho_\beta(x')\} \tag{A·10}$$

must comprise the terms such as

$$\bar{\psi}(x)O_\alpha\psi(x)\langle\bar{\psi}(x')O_\beta\psi(x')\rangle_0. \tag{A·11}$$

Since in the case of the electron interacting with the electromagnetic field the vacuum expectation value of $\rho_\alpha(x)$ vanishes identically by the charge symmetry reasons, we used to omit the terms like (A·11) from the beginning, but so long as such special condition does not exist we ought to consider the processes like Fig. 2 in Dyson formalism.

Thus the difficulty about the "vacuum polarization type" pointed out by Sawada[8], Yukawa-Umezawa[4] and Epstein[9] is dissolved again.

Similar circumstances occur in the one particle correction of $\varkappa^2\int Q_\alpha Q_\alpha dv$ (see Fig. 4).

Fig. 1

Fig. 2

Fig. 3

Fig. 4

References

1) Private communication from Dr. A. Pais to Dr. S. Tomonaga.
A. Pais and S. T. Epstein, Rev. Mod. Phys. **21** (1949), 445.
2) J. Schwinger, Phys. Rev. **75** (1949), 651.
3) R. Kawabe and H. Umezawa, Prog. Theor. Phys. **4** (1949), 468.
4) J. Yukawa and H. Umezawa, ibid. **6** (1951), 112.
5) S. Sakata, H. Umezawa and S. Kamefuchi, ibid. **7** (1951), 377.
6) W. Pauli, Rev. Mod. Phys. **13** (1941), 203.
7) Z. Koba, Prog. Theor. Phys. **5** (1950), 696.
8) K. Sawada, ibid. **5** (1950), 117.
9) S. T. Epstein, ibid. **6** (1951). 441.

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On the Cosmic-Ray Bursts Underground

—— *The Interaction of π-meson with Nucleon* ——

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A high energy μ-meson can produce π-meson, when it collides with a nucleon by its electromagnetic field. The energy dependency of the cross section for this process is analysed from the view point of the perturbation method including higher order corrections, when only the pseudo-scalar (direct) coupling of π-meson with nucleon is assumed. Next, retaining the character of the cross section thus obtained, we assume a phenomenological cross section for this process and apply it to the analysis of cosmic-ray burst underground. Then it is found that the consistency between the theory and the experiment seems not to be attainable, when only the direct coupling is taken into account. However, some remarks are given on the information indicated by the burst experiment underground, before a definite conclusion is deduced.

§ 1. Introduction

Recent researches have shown that the charged π-meson is of the pseudo-scalar type. For the further development of π-meson theory, it seems to be important to know about the nature of interaction of π-meson with nucleon. As is well known, the meson theory suggests two modes of interaction between the π-meson and the nucleon, that is, the pseudo-scalar (direct) and the pseudo-vector (derivative) coupling. To analyse which of these two interactions is actually realized is interesting from the view point of the present field theory. As the renormalization method has been succeeded in the formation of a consistent quantum electrodynamics though its substantial defect is still remained to be solved, it is very interesting to investigate whether the above method is also applicable or not to the region outside the electromagnetic phenomena.

It has already been pointed out that the Fermi interaction in the β-decay process and the derivative coupling in the pseudo-scalar meson theory leads to the failure of the renormalization method.[1)2)] However, Fermi interaction may be replaced by another interaction which comes out through the mediation of other field (e.g. a heavy meson field) including only the first kind interaction. On the other hand, while the derivative coupling of pseudo-scalar meson theory seems to be partly supported by the scattering experiment of π-meson with nucleon, this information is not quite conclusive, if the higher order correction and the isobar states of nucleon are taken into account. In such situation it may be necessary to study whether all phenomena which happen in nature can be describable by only the interaction of the first kind or not.

Since the analysis of the validity of renormalization method is primarily based on the investigation about the order of the divergence, it is quite natural that we take the high energy phenomenon in order to analyse this problem. We shall study the contribution of π^0-meson to the cosmic-ray bursts underground which is caused by the collision of high energy μ-meson with nucleon. A high energy collision of μ-meson with nucleon leads to the production* of several charged mesons as well as neutral mesons, which gives mixed shower. As is well known, the interaction of μ-meson with nucleon is only electromagnetic and so this process would explicitely show the character of the coupling between nucleon and π-meson. Our purpose is to investigate whether such a weak character of interaction as pseudo-scalar coupling can give a considerable frequency of the mixed shower consistent with the experiment or not. We shall begin with only direct coupling of π-meson with nucleon.

First, the problem how the cross section and the energy loss in this process depend on the incident μ-meson energy, is studied by means of the perturbation method taking account of the higher order correction (§ 2). Next, according to thus obtained qualitative results, the phenomenological cross section is assumed (§ 3) and this is applied to the analysis of the cosmic-ray bursts underground (§ 4). In order to make the comparison of the theory with the experiment clear, some remarks are given about the experiment of the cosmic-ray burst underground.

§ 2. The π-meson production by the μ-meson

The results in the lowest order perturbation calculation have already been obtained by Fukuda, Fujimoto and Koshiba[3] and Fujimura.[4] When only the pseudo-scalar coupling is used as the interaction of π-meson with nucleon, the cross section and energy loss in this process depend only logarithmicaly on the incident μ-meson energy and this dependency is caused only by the character of the interaction used**, that is, direct interaction, and does not depend on whether the π-meson is charged or neutral. In fact, if we use the pseudo-vector coupling and the non-relativistic approximation,[5] the obtained energy loss depends linearly on the incident energy because of the fact that the used interaction includes derivatives, while the relativistic calculation in the lowest order, of course, leads to the same result due to the equivalence theorem, irrespective of the coupling used.

Now we shall inquire about the modification in the cross section, especially in its energy dependency, when higher order correction of direct coupling is taken into account. In high energies, the energy dependency of the cross section is determined by the momentum dependency of the interaction used.[6][7]

The case (*i*). *One* π*-meson in final state*

In this case, we should study only the modification of the effective interaction caused

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* In the following, we call this as μ- π-process.

** This statement is supported by the fact that the energy dependency remains unchanged when the scalar coupling is used as the interaction of π-meson with nucleon.

by the higher order correction. According to Sakata, Umezawa and Kamefuchi,[1] the momentum dependency of the effective interaction cannot exceed that of the initially taken after an appropriate renormalization if only direct coupling is used in the higher order calculation. Accordingly, the energy dependency of the cross section remains effectively unchanged.

The case (ii). Two or more π-mesons in final state

At first we take the case of two π-mesons in final state. According to Feynman diagram [see Fig. 1] the differential cross section differes from that in the case of one π-meson in final state by the factor,

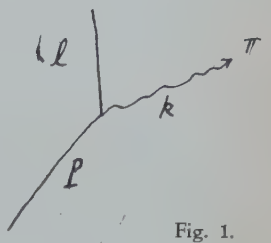

Fig. 1.

$$d\sigma = \cdots\cdots \frac{d\boldsymbol{k}}{\epsilon} \left| \gamma_5 \frac{i\gamma P + M}{P^2 + M^2} \cdots \right|^2 \qquad (1)$$

when one of the diagrams is taken out. ϵ and $\boldsymbol{k}$ are the energy and the momentum of the secondary emitted π-meson, respectively. P and M are the linear combination of energy-momentum 4-vectors of the associated particles and the nucleon mass.....indicates the factors which appear in the case of one π-meson in final state. We are interested in only the momentum (or energy) dependency of $d\sigma$, and so the fact that.....is different from the reality can be neglected because this difference leads to no different energy dependency of $d\sigma$. We obtain,

$$d\sigma = \cdots\cdots \frac{d\boldsymbol{k}}{\epsilon} \left| \frac{-P^2 + M^2}{(P^2 + M^2)^2} \right| \cdots\cdots \Big|^2, \qquad (2)$$

where = indicates the equality of the momentum dependency in each term. When the incident μ-meson energy E_0 is very large ($E_0 \gg M$, $\varkappa = \pi$-meson mass), the contribution of the integral on $d\boldsymbol{k}$ comes from the region $|\boldsymbol{k}| \quad \epsilon = o(E_0)$. [$o$ indicates the order of magnitude.]

Let us take into account the integral,

$$\frac{d\boldsymbol{k}}{\epsilon} \left| \frac{1}{P^2 + M^2} \right| = k dk \sin\theta \, d\theta \, d\varphi \left| \frac{1}{P^2 + M^2} \right|. \qquad (3)$$

Separating ϵ and $\boldsymbol{k}$ from others in P, we obtain

$$-(P^2 + M^2) = (l_4 + \epsilon)^2 - (\boldsymbol{l} - \boldsymbol{k})^2 - M^2 = l_4^2 - l^2 - 2k(l_4 - l\cos\theta). \qquad (4)$$

l_4 and $\boldsymbol{l}$ are respectively the linear combinations of the energies and momenta of associated particles excepting those of the secondary emitted π-meson. Then, (3) is integrated on $d\cos\theta$ as,

$$k\, dk\, d\varphi \int d\cos\theta \, \frac{1}{2k(l_4 - l\cos\theta) - F^2}; \quad F^2 = l_4^2 - l^2$$

$$= d\varphi \, dk/2l \cdot [\text{Log. Term}]. \qquad (5)$$

Rewriting l as $|\boldsymbol{P} - \boldsymbol{k}|$, we find that the integral on dk in (5) leads to the logarithmic dependent term.

Accordingly, the modification of the cross section and the energy loss in the $\mu-\pi$ process is at most the multiplication by the logarithmically dependent term on the incident energy, compared with that in the case of one π-meson in final state. The above discussions are valid in each diagram involved and also valid in the cross term contribution of them.* When three or more π-mesons are in final state, the mentioned deduction is applicable step by step.†

§ 3. Phenomenological treatment

In the preceding paragraph we have studied the general feature of the energy dependency of the $\mu-\pi$ cross section when only direct coupling of π-meson with nucleon is assumed. However, the value of coupling constant is remained as arbitrary. In the present situation of the meson theory, we may take it such as to give the total cross section of $\mu-\pi$ process consistent with the observed value. Then the differential cross section with which μ-meson of energy E_0 produces π-meson of energy between E and $E+dE$ is generally given by,

$$dE\sigma(E_0,\ E)=\phi_0\sum_{\nu}a_\nu E^{-\nu}\,dE\ ;\ \nu\geq 2, \tag{6}$$

if only the direct coupling is assumed to exist between the nucleon and the π-meson. ϕ_0 is the appropriate constant with the dimension of cross section. a_ν may depend on E_0 only logarithmically. $\nu\geq 2$ is the condition that the total cross section and the energy loss in $\mu-\pi$ process depend on E_0 only logarithmically. We take nucleon mass as the lower limit of the integral (6), though energetically it is π-meson mass. This choice is required in order not to underestimate the contribution from π^0-meson to burst production. That is, to make the lower limit greater leads to larger value of the mean energy transmitted to π^0-meson. In (6) $\nu=2$ is the value which gives the largest mean energy,

$$\bar{E}=\int_M^{E_0}a_\nu\bar{E}^\nu dE\cdot E\Big/\int_M^{E_0}a_\nu\bar{E}^\nu dE$$
$$=M\log(E_0/M)^{**}.$$

Taking only this term into account, we obtain

$$dE\sigma(E_0,\ E)=\phi_0\{\log(E_0/M)\}^s M\cdot dE/E^2\ ;\ E\geq M, \tag{7}$$

where $\phi_0\{\log(E_0/M)\}^s$ is put to give the total cross section of $\mu-\pi$ process consistent with the experiment. At $E_0=15$ Bev, which corresponds to the mean energy of μ-meson at 60 m H_2O underground, $\phi_0\{(\log E_0/M)\}^s=2\mu b$. A half of energy emitted with the

* In this deduction, we assume the μ-meson to be spin 1/2 particle. The qualification in this paragraph is essentially unchanged, if μ-meson is Bose particle with spin 0.

† On the more general discussion about the meson production in the nucleon-nucleon collision, see ref. (6).

** According to Fukuda, Fujimoto and Koshiba,[3] $\bar{E}\simeq(M/3)\log(E/M)$. Our larger value $\bar{E}$ is followed by the fact that we take the differential cross section such as to give maximum energy transfer.

cross section (7) is transmitted to π^0-meson which decays into two photons. Then the spectrum of the photon with energy between k and $k+dk$ is obtained as,

$$dk \cdot \sigma(E_0, k) = \phi_0 \{\log(E_0/M)\}^s M(1-k^2/E_0^2)dk/k^2. \quad (8)$$

§ 4. Cosmic-ray burst underground

The $\mu-\pi$ process contributes to the burst production underground, where the μ-meson is the main component of cosmic ray. The high energy collision of μ-meson with nucleus may give the simultaneous production of several π-mesons, resulting to the mixed shower. If this process is "plural", then the spectrum (8) will be somewhat modified. This modification, however, may be effective only to lower the mean energy transmitted to π^0-meson and we do not take any secondary nuclear effect into account in (8), in order to obtain the upper limit of the π^0-meson contribution to burst.

The mixed cosmic-ray burst underground has already been observed by George and Trent[8] who have found several penetrating particles under 15 cm Pb simultaneously with the burst production in ionization chamber. They have atributed this phenomenon to the mixed shower caused by $\mu-\pi$ process and found the observed frequency to be reasonable if the energy loss in $\mu-\pi$ process depends linearly on the incident μ-meson energy in contrast with that obtained in the preceding paragraph.

We shall analyse this phenomenon in order to make clear whether the obtained spectrum (8) can give the experimental result reasonably or not. The following analysis is the same as that used by Christy-Kusaka[9] and we give only the calculated results. However it should be noted that the recent study[10] on the cascade theory indicates the current theory to be insufficiently accurate and so we have estimated the relative frequency of burst caused by $\mu-\pi$ process to that caused by Bremsstrahlung of μ-meson. The obtained results at 60 m H_2O underground are presented in Table I. S and β are the size of burst and the critical energy in the cascade theory respectively and in our case $\beta \sim 15$ Mev. $R_\pi(1)$ and $R_\pi(3)$ corresponds to $s=1$ and $s=3$ in (8) respectively. R_π is the case where energy loss in $\mu-\pi$ process is assumed to be the same as that in Bremsstrahlung, which is analogous to that used by George and Trent in their analysis.

Table I. Burst frequency normalized to those caused by Bremsstrahlung

Burst size=(Bev)	0.5	1.0	2.0	4.0
R(knock-on)	0.76	0.46	0.23	0.12
$R_\pi(1)$	0.0080	0.0062	0.0040	0.0022
$R_\pi(3)$	0.012	0.011	0.0080	0.0072
R_π	0.057	0.057	0.057	0.057
R_{exp}	0.1	0.1	0.1	0.1

Before the discussion on Table I is made we shall give a crude estimation on the

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R_π (3) corresponds to the case when the total cross section of $\mu-\pi$ process varies as $\propto (\log E_0)^3$ and results in that the observed cross section at 60 m H_2O underground should be larger by a factor 4.5 than that at 20 m H_2O. The experiment seems to show a factor less than 2 at these two depths, indicating definitely $s < 3$ in (8).

correlation of βS with the observed burst size $n=20\sim150$ given in G.T. Taking account of the lateral spread of cascade electron, we find the number n of electrons which strike the ionization chamber to be 1/3.5 times smaller than the total number.[11] Then the observed number $n=50$ corresponds to $\beta S=2.5$. As is clear from Table I, we find that the assumed spectrum (8) gives the inconsistently small frequency compared with the experimental value which, in over all size, amounts to about 10% of the frequency caused by μ-mesons Bremsstrahlung. From the comparison of $K_\pi(1)$ and $K_\pi(3)$, we can see that the modification of the cross section by some logarithmically dependent factor does not lead to any essential change in frequency.

On the other hand, we should note that the energy dependency of the differential cross section taken as same as that given by Bremsstrahlung gives a nearly consistent result. G. T. have used the cross section with the same character of energy dependency, which is obtained by Williams-Weizsaecker's method from photo-meson production. The good agreement of our calculated result with those obtained by them shows that the contributions of process to burst phenomena depend essentially on only the qualitative nature of energy dependency of its cross sections, when once total cross section is fitted.

§ 5. Some remarks on the analysis

In the preceding analysis of mixed shower, we have neglected the contribution of nuclear component to the burst size. When $\mu-\pi$ process occurs, nuclear components may be produced together with π-mesons. The slow protons in these components increase the apparent burst size caused by π^0-meson. We have estimated this contribution according to phenomenological nuclear cascade theory[12] and found that it amounts at most to 20% of burst size caused by π^0-meson. The corresponding burst frequency increases at most by a factor 1.5 and our conclusion obtained in last paragraph remains unchanged.

Next we shall discuss on the experimental results. In the experiment by G. T., counters which record penetrating particles are set under 15 cm Pb, above which ionization chamber is set. The low energy photon in the tail of the cascade which gives burst in ionization chamber can strike the counter tray under 15 cm Pb with a considerable probability, and this phenomenon may be apparently attributed to the mixed shower. We have done a crude estimation on the contribution of the low energy photon. According to Greisen[13] the probability that a photon of cascade which gives burst of size $n=20\sim150$ in ionization chamber strikes the counter under 15 cm Pb amounts to $20\sim80\%$. If the counter striked by the photon (in the cascade initiated by μ-meson's Bremsstrahlung) is apart from the counter which the incident μ-meson penetrates, we may take this phenomenon as mixed shower caused by $\mu-\pi$ process. In order to estimate what fractions of these photons strike the counter, it should be necessary to develop more elaborate cascade theory in shower tail. We should remark only that the mixed burst observed by G. T. is not all attributed to $\mu-\pi$ process. Accordingly it may be necessary that the nature of the particles that strike the counter under 15 cm Pb is investigated directly with the cloud chamber. The use of more thick absorber may also serve to exclude the low energy photon's contributions.

Some evidence against the effect of low energy photon seems to be presented in the experiment by G. T. In the size frequency curve given by G. T. the exponent of the curve caused by μ-meson Bremsstrahlung is somewhat smaller ($=1.6$) than that attributed to $\mu-\pi$ process ($=1.75$). If the latter is caused by the low energy photon of the cascade tail initiated by μ-meson's Bremsstrahlung, it should be flatter than the former, because the photon's contribution should increase with the burst size.

§ 6. Conclusion

We have analysed the qualitative nature of energy loss caused by $\mu-\pi$ process, when only the pseudo-scalar coupling is assumed as the interaction between π-meson and nucleon. In this calculation we have neglected the Pauli-moment of nucleon. If the anomalous magnetic moment of nucleon is attributed to the interaction of π-meson with nucleon, the qualitative nature obtained in § 2 remains unchanged. The experiment on burst underground seems to indicate that the above obtained nature of energy loss in $\mu-\pi$ process is quite inconsistent and a stronger interaction is necessary between π-meson and nucleon than the pseudo-scalar interaction. However it should be noted that the more elaborate experiment is necessary before the definite conclusion is attained.

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1) S. Sakata, H. Umezawa and S. Kamefuchi, Phys. Rev. **84** (1952), 154; Prog. Theor. Phys. **7** (1952), 377. We shall follow their classification of interaction type. Interactions are called as the 1st kind or the second kind according to whether they are renormalizable or not.
2) S. Kamefuchi, Prog. Theor. Phys. **6** (1951), 175.
3) H. Fukuda, Y. Fujimoto and M. Koshiba, Prog. Theor. Phys. **6** (1951), 815.
4) J. Fujimura, Annual meeting of Phys. Soc. Japan Oct. (1951).
5) I. N. Sneddon and B. F. Touschek, Proc. Roy. Soc. **199A** (1950), 352.
6) H. Umezawa, S. Kamefuchi and Y. Takahashi, Phys. Rev. **85** (1952), 505.
7) H. Umezawa, Prog. Theor. Phys. **7** (1952), 551.
8) E. P. George and P. T. Trent. Proc. Phys. Soc. **64** (1951), 733. We call this as G. T.
9) R. F. Christy and S. Kusaka, Phys. Rev. **59** (1941), 414.
10) J. Nishimura and K. Kamata, Prog. Theor. Phys. **5** (1950), 889.
11) H. Komori, K. Miyanaga and S. Ogawa, Prog. Theor. Phys. **7** (1952), 122.
12) S. Hayakawa, unpublished.
13) K. Greisen, Phys. Rev. **75** (1949), 1072.

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Some Consequences of Gauge Invariance

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A simple theorem is stated to expand the matrix element for a process concerning any number of photons or external electromagnetic fields into the independent gauge invariant terms. It turns out that the number of such terms is uniquely determined by the initial and final states of the process, regardless of the intermediate states and the type of interaction. We have, for example, 4, 14, and 10 independent gauge invariant terms for the production of spin 0 and 1 mesons by photons and the Compton scattering, respectively. Some of the well-known absolute selection rules for meson decays can be also derived from this gauge invariant expansion theorem.

§ 1. Introduction

In their recent works on the production of spinless mesons by photons,[1),**] Koba *et al.* have shown that the requirement of gauge invariance greatly simplified the evaluation and made facile the analysis of the results. In fact they developed the enormous number of matrix elements into only four independent gauge invariant terms irrespective of the order of approximation. Their conclusion was a direct consequence of i) Lorentz invariance, ii) gauge invariance, iii) energy-momentum conservation, iv) spinless field for the meson, and v) Dirac equation for the nucleon, and thus it mattered only about the initial and final states of the process but not about the method of calculation. Such a procedure can therefore be applied *mutatis mutandis* to other cases involving one or more photons or external electromagnetic fields. However, since their method itself is very special and seems inconvenient to apply to other processes, its reexamination is desirable.

It is the aim of this paper to observe the gauge invariance from the most general points of view and present a method to expand complex matrix elements into their fundamental gauge invariant terms. We shall show in § 2 that a simple consideration indeed affords us such a prescription which is far more concise than theirs and in addition widely applicable. In the next section, the gauge invariant expansion theorem of the matrix elements is given, according to which it turns out that the number of gauge invariant terms is unambiguously determined by the process, not depending on the method of calculation. We have, for example, 4, 14, and 10 such terms for the production of spin 0 and 1 mesons by photons and the Compton scattering, respectively. In § 4 the possibilities are discussed for utilizing this theorem to derive the absolute selection rules for meson decay. However, as might be expected, the selection rules are obtained only for certain simple cases.

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** The paper by Koba, Kotani and Nakai (Prog. Theor. Phys. **6** (1951), 849) will be referred to as (K.K.N.).

§ 2. Gauge invariance factor

We shall use in what follows the momentum representation for the sake of practical purpose. The general matrix element M between given states is specified by the operator product χ and the c-number coefficient R:

$$M=R\chi. \tag{1}$$

Here χ is a product in correct order of the Fourier amplitudes of the free operators and the unquantized external fields. R is to be expressed in terms of given four-momenta of participating particles and fields and also γ-matrices.* Since M is invariant under a Lorentz transformation, the transformation property of R is determined by that of χ, that is to say, it is completely characterized by the initial and final states of the transition.

Now since we are interested in a photon or an external electromagnetic field, (1) may be expressed in the form,

$$M=R_\mu(\boldsymbol{k},\cdots\cdots)A_\mu(\boldsymbol{k})\chi', \tag{2}$$

by extracting an electromagnetic potential A_μ under consideration from χ. $\boldsymbol{k}$ is a given four-momentum which satisfies $\boldsymbol{k}^2=0$ when A_μ is concerned with a free photon. R_μ, here, behaves as if it were a four-vector with a suffix μ corresponding to the polarization of A_μ, it may have of course any other hidden index representing further degrees of freedom.

The invariance of M under a gauge transformation of A_μ requires[2],**

$$i\,k_\mu R_\mu=0, \tag{3}$$

which makes it possible to rewrite (2) as

$$M=R_\mu A_\mu(\boldsymbol{k})\chi'=(\delta_{\mu\alpha}+F_\mu\cdot ik_\alpha)R_\alpha A_\mu(\boldsymbol{k})\chi', \tag{2'}$$

with F_μ an arbitrary non-singular function of the states. If one puts $F_\mu=if_\mu/\boldsymbol{fk}$, (2') is disguised again into

$$M=R_\mu A_\mu(\boldsymbol{k})\chi'=\left(\delta_{\mu\alpha}+\frac{if_\mu}{\boldsymbol{fk}}\cdot ik_\alpha\right)R_\alpha A_\mu(\boldsymbol{k})\chi', \tag{2''}$$

f_μ being a simple function chosen conveniently for each case. Then we can directly see the gauge invariance of M because of $ik_\mu(\delta_{\mu\alpha}+if_\mu/\boldsymbol{fk}\cdot ik_\alpha)=0$ independent of R_α. This means that the requirement of gauge invariance is fulfilled in an individual Feynman diagram. But the relation (3) is valid only if one treats *en bloc* all diagrams that belong to the same "gauge invariant class".[2] At first sight these two statements appear to contradict with each other. The doubt is, however, dispelled when one considers (2'') as obtained by adding (2) appropriate terms which totally give zero and then by rearranging

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* The use of β-formalism does not require any essential alteration of the arguments.

** As is well-known, this relation in momentum space is not always satisfied if there exist charged closed loops in the sense of the Feynman diagram, whilst the similar one in coordinate space always holds. Assuming, however, that such an ambiguity might be removed by some procedure, we may start from (3).

the matrix elements so as to make clear their gauge invariance, the process being indeed performed at a stretch by merely multiplying a factor $(\delta_{\mu\alpha}+if_\mu/\boldsymbol{fk}\cdot ik_\alpha)$. This factor is called hereafter a *G-factor* for $A_\mu(\boldsymbol{k})$ and denoted by $G_{\mu\alpha}(\boldsymbol{k})$. We have thus (2″) as a concrete presentation of (3).

Now, it is very easy to extend this procedure to the cases involving two or more A_μ's and get the gauge invariant matrix elements with respect to all A_μ's concerned. The matrix element of a process which contains n A_μ's is, as an extension of (2),

$$M=R_{\mu\nu\cdots\omega}(\boldsymbol{k}_1, \boldsymbol{k}_2, \cdots, \boldsymbol{k}_n, \cdots)A_\mu(\boldsymbol{k}_1)A_\nu(\boldsymbol{k}_2)\cdots A_\omega(\boldsymbol{k}_n)\chi^{(n)}. \tag{4}$$

The requirements of gauge invariance,

$$ik_{1\mu}R_{\mu\nu\cdots\omega}=ik_{2\nu}R_{\mu\nu\cdots\omega}=\cdots=ik_{n\omega}R_{\mu\nu\cdots\omega}=0, \tag{5}$$

lead to M of a desired form:

$$M=G_{\mu\alpha}(\boldsymbol{k}_1)G_{\nu\beta}(\boldsymbol{k}_2)\cdots G_{\omega\lambda}(\boldsymbol{k}_n)R_{\alpha\beta\cdots\lambda}A_\mu(\boldsymbol{k}_1)A_\nu(\boldsymbol{k}_2)\cdots A_\omega(\boldsymbol{k}_n)\chi^{(n)}, \tag{4′}$$

where the j-th G-factor $G_{\rho\zeta}(\boldsymbol{k}_j)$ stands for $(\delta_{\rho\zeta}+if_{j\rho}/\boldsymbol{f}_j\boldsymbol{k}_j\cdot ik_{j\zeta})$.

We shall apply our method, by way of examples, to the $\gamma-\pi$ production and the Compton scattering in their lowest order of weak coupling approximation.

1. *The production of spinless mesons by photons*

For the process $N+\gamma\rightarrow N'+\pi$, its matrix element in *ef*-approximation is, apart from an inessential factor for the present purpose, given by

$$M=ef_i\bar{\psi}(\boldsymbol{p}')\varphi_i(\boldsymbol{l})R_{\mu i}(\boldsymbol{k}, \boldsymbol{l}, \boldsymbol{p}, \boldsymbol{p}', \boldsymbol{\gamma})\psi(\boldsymbol{p})A_\mu(\boldsymbol{k}), \tag{6}$$

with

$$\begin{aligned}R_{\mu i}(\boldsymbol{k}, \boldsymbol{l}, \boldsymbol{p}, \boldsymbol{p}', \boldsymbol{\gamma})=&\gamma_5'\tau_i S_F(\boldsymbol{p}+\boldsymbol{k})\gamma_\mu\tau_P+\gamma_\mu\tau_P S_F(\boldsymbol{p}'-\boldsymbol{k})\gamma_5'\tau_i\\&+\gamma_5'(\tau_1\varepsilon_{2i}-\tau_2\varepsilon_{1i})\cdot 2l_\mu\Delta_F(\boldsymbol{l}-\boldsymbol{k}),\end{aligned} \tag{7}$$

where $\boldsymbol{k}$, $\boldsymbol{p}$, $\boldsymbol{p}'$ and $\boldsymbol{l}$ represent the four-momenta of the incident photon, the initial and final nucleon, and the produced meson, respectively; $\boldsymbol{e}_1=(1, 0, 0, 0)$ and $\boldsymbol{e}_2=(0, 1, 0, 0)$ are two unit vectors in the four-dimensional τ-spin space with $\tau_4=1$; the summation over i is to be taken from 1 to 4. S_F and Δ_F are familiar functions indicating the propagation of nucleon and meson. $\gamma_5'=1$ for scalar φ_i, and $=i\gamma_5$ for pseudoscalar φ_i.

Multiplied a G-factor $G_{\mu\alpha}(\boldsymbol{k})$, in which one puts conveniently $\boldsymbol{f}=\boldsymbol{p}$, (7) becomes

$$\begin{aligned}R_{\mu i}=G_{\mu\alpha}R_{\alpha i}=&(i\boldsymbol{\gamma k})\gamma_\mu\gamma_5'\left[\frac{\tau_i\tau_P}{2\boldsymbol{pk}}-\frac{\tau_P\tau_i}{2\boldsymbol{p'k}}\right]\\&+2i\left(l_\mu-\frac{p_\mu}{\boldsymbol{pk}}\cdot\boldsymbol{kl}\right)\gamma_5'\left[\frac{\tau_P\tau_i}{2\boldsymbol{p'k}}+\frac{i(\tau_1\varepsilon_{2i}-\tau_2\varepsilon_{1i})}{2\boldsymbol{kl}}\right].\end{aligned} \tag{8}$$

We can thus readily develop the matrix element in terms of two gauge invariant terms, $(i\boldsymbol{\gamma k})\gamma_\mu\gamma_5'$ and $i(l_\mu-p_\mu/\boldsymbol{pk}\cdot\boldsymbol{kl})\gamma_5'$, with coefficients not containing γ-matrices. This result is of course the same as obtained by Koba et al.[1]

2. *The Compton scattering*

The matrix element in e^2-approximation is

$$M=e^2\psi(\boldsymbol{p}')A_\nu(\boldsymbol{k}')R_{\mu\nu}(\boldsymbol{k},\boldsymbol{k}',\boldsymbol{p},\boldsymbol{p}',\gamma)A_\mu(\boldsymbol{k})\psi(\boldsymbol{p}), \tag{9}$$

with

$$R_{\mu\nu}(\boldsymbol{k},\boldsymbol{k}',\boldsymbol{p},\boldsymbol{p}',\gamma)=\gamma_\nu S_F(\boldsymbol{p}+\boldsymbol{k})\gamma_\mu+\gamma_\mu S_F(\boldsymbol{p}-\boldsymbol{k}')\gamma_\nu, \tag{10}$$

S_F, here, being the propagation function for electron. The use of two G-factors $G_{\mu\alpha}(\boldsymbol{k})$ and $G_{\nu\beta}(\boldsymbol{k}')$, with $\boldsymbol{f}=\boldsymbol{f}'=\boldsymbol{p}$, allows one to get the gauge invariant expansion of (10):

$$\begin{aligned}R_{\mu\nu}(\boldsymbol{k},\boldsymbol{k}',\boldsymbol{p},\boldsymbol{p}',\gamma)&=G_{\mu\alpha}(\boldsymbol{k})G_{\nu\beta}(\boldsymbol{k}')R_{\alpha\beta}\\&=\frac{1}{2\boldsymbol{p}\boldsymbol{k}}\Big(\gamma_\nu+\frac{i\boldsymbol{p}_\nu}{\boldsymbol{p}\boldsymbol{k}'}\cdot i\gamma\boldsymbol{k}'\Big)(i\gamma\boldsymbol{k})\gamma_\mu+\frac{1}{2\boldsymbol{p}\boldsymbol{k}'}\Big(\gamma_\mu+\frac{i\boldsymbol{p}_\mu}{\boldsymbol{p}\boldsymbol{k}}\cdot i\gamma\boldsymbol{k}\Big)(i\gamma\boldsymbol{k}')\gamma_\nu.\end{aligned} \tag{11}$$

§ 3. Gauge invariant expansion theorem

In preceding section we have shown that any matrix element which satisfies the requirement of gauge invariance can easily be written down by the use of G-factor in an obviously gauge invariant form. We shall here study in detail the general features of such an expansion in order to recognize their significance.

As the c-number part R in (1) is eventually expressed by external four-momenta and γ-matrices only, we obtain

$$R=\sum_{l,m}c_{lm}(\Lambda_l\,T_m). \tag{12}$$

Here T_m's are all possible quantities with the same transformation property as R that are built of the available four-momenta and γ-matrices and independent of one another, so that they have just the same suffices as R. $\Lambda_1=1$ always, while for $l\neq 1$ Λ_l is either a product of any number of scalar factors $(\gamma\boldsymbol{p}_1)$, $(\gamma\boldsymbol{p}_2)$, $\cdots\cdots$, where $\boldsymbol{p}_1$, $\boldsymbol{p}_2$, $\cdots$ are external four-momenta, or $\Lambda_l=0$ according as R does or does not contain γ-matrices. As will be seen below the order of Λ_l and T_m is inessential for the present considerations even if they were non-commutative. c_{lm} is an invariant quantity constructed only by external four-momenta, not containing γ-matrices. The summation is to be taken over all possible combinations of Λ_l and T_m.

Given any states, between which a transition takes place, one can easily set up all possible T_m's from the transition property of R. We shall denote the number of such T_m's by $N(T)$. On the other hand, from the properties of γ-matrices the type of Λ_l's is restricted: each Λ_l does not contain two or more identical factors and in addition one needs take no notice of the order of different factors in individual Λ_l. Furthermore, the conservation law of energy-momentum and the equations of motion for the free particles diminish the number of possible Λ_l's. We shall denote the number of thus obtained Λ_l's by $N(\Lambda)$. Therefore the summation in (12) is over $N(\Lambda)N(T)$ independent terms $(\Lambda_l\,T_m)$'s. Thus we can see that the form as well as the number of the products $(\Lambda_l\,T_m)$'s are completely characterized by the initial and final states alone without need

of any other specification about the intermediate states, the mode of coupling between interacting particles, and so on. The c_{lm}'s in (12), however, depend how to calculate R, that is, they have different forms according to the formalism adopted and the order of approximation.

As a result of the analysis so far, we conclude that R can always be expanded in terms of the definite number of terms $(\Lambda_l T_m)$'s characteristic of the process, with c_{lm}'s as coefficients. This conclusion is rather trivial but very important.

When the process is concerned with photons or external electromagnetic fields, $A_\mu(\boldsymbol{k})$'s, we may conveniently introduce the G-factors to get the gauge invariant matrix element with regard to all $A_\mu(\boldsymbol{k})$'s. The G-factor then acts only on the characteristic part $(\Lambda_l T_m)$, correctly speaking on T_m, of R and change it into a gauge invariant term $(\Lambda_l G T_m)$, but leave c_{lm} as it stands. Therefore the introduction of G-factors does not essentially modify the general expansion theorem of the matrix element stated above. On the contrary, it makes the theorem useful because an appropriate choice of the arbitrary function $\boldsymbol{f}$ in the G-factor considerably reduces $N(T)$, though $N(\Lambda)$ remains unchanged: $N(GT) < N(T)$. Thus we get the gauge invariant expansion theorem: for a gauge invariant matrix element $M = R\chi$, R can always be developed in terms of $N(\Lambda)N(GT)$ independent gauge invariant terms $(\Lambda_l G T_m)$'s, namely,

$$R = GR = \sum_{l,m} c_{lm}(\Lambda_l G T_m), \tag{13}$$

and this number is also uniquely determined by the initial and final states of the process alone, regardless of the intermediate states and the type of interaction.

We shall apply this theorem again to the $\gamma-\pi$ production and the Compton scattering. In this time, however, we do not make any assumption about the formalism and the approximation.

1. *The production of spin 0 mesons by photons*

The matrix element for this process is, as a generalization of (6), given by

$$M = \bar{\psi}(\boldsymbol{p}')\varphi(\boldsymbol{l})R_\mu(\boldsymbol{k}, \boldsymbol{l}, \boldsymbol{p}, \boldsymbol{p}', \gamma)\psi(\boldsymbol{p})A_\mu(k). \tag{14}$$

Here R_μ behaves as vector or pseudovector according as φ is scalar or pseudoscalar, which is perfectly described by inserting γ_5' in R_μ because it needs no special notice at the nucleon closed loop,* so that, writing $R_\mu = \gamma_5' R_\mu'$, R_μ' has the transformation property of ordinary vector in both cases.

Now the gauge invariant expansion theorem gives,

$$\begin{aligned} R_\mu(\boldsymbol{k}, \boldsymbol{l}, \boldsymbol{p}, \boldsymbol{p}', \gamma) &= \gamma_5' G_{\mu\alpha}(\boldsymbol{k}) R_\alpha'(\boldsymbol{k}, \boldsymbol{l}, \boldsymbol{p}, \boldsymbol{p}', \gamma) \\ &= \sum_{l,m} c_{lm}(\Lambda_l G_{\mu\alpha} T_{\alpha m} \gamma_5'). \end{aligned} \tag{15}$$

* From the *Spur* over the nucleon closed loop, with which odd number of pseudoscalar mesons are coupled, there appears a pseudoscalar quantity, which, however, may be expressed as a certain linear combination of scalar quantities multiplied by γ_5. See the foot note on p. 857 of (K.K.N.).

Eliminating first $\boldsymbol{p}'$ by the conservation law, all possibilities of $T_{\alpha m}$ are four in number: k_α, p_α, l_α and γ_α, the former two of which may be disregarded because $G_{\mu\alpha}k_\alpha=0$ which follows from $\boldsymbol{k}^2=0$ and $k_\mu A_\mu(\boldsymbol{k})=0$, and because $G_{\mu\alpha}p_\alpha=0$ if one chooses $\boldsymbol{f}=\boldsymbol{p}$ as an arbitrary function in $G_{\mu\alpha}$, so that $N(G_{\mu\alpha}T_\alpha)=2$. Next, eliminating $\boldsymbol{l}$ by the conservation law, $\boldsymbol{p}$ and $\boldsymbol{p}'$ by the equations of motion, we may take only 1 and $(i\boldsymbol{\gamma}\boldsymbol{k})$ as Λ_l's, so that $N(\Lambda)=2$. Therefore (15) becomes the summation over $2\times 2=4$ independent gauge invariant terms:

$$R_\mu=G_{\mu\alpha}\{c_{11}l_\alpha+c_{12}\gamma_\alpha+c_{21}(i\boldsymbol{\gamma}\boldsymbol{k})l_\alpha+c_{22}(i\boldsymbol{\gamma}\boldsymbol{k})\gamma_\alpha\}\gamma_5', \tag{16}$$

where $G_{\mu\alpha}=(\delta_{\mu\alpha}+ip_\mu/\boldsymbol{p}\boldsymbol{k}\cdot ik_\alpha)$, c's are the invariant function of $\boldsymbol{p}$, $\boldsymbol{k}$, and $\boldsymbol{l}$, and essentially depend on the energy of the incident photon and the angle (or the energy) of the emitted meson. (16) shows that R_μ in this case always can be expanded in terms of only four fundamental gauge invariant terms*, $(l_\mu-p_\mu/\boldsymbol{p}\boldsymbol{k}\cdot\boldsymbol{k}\boldsymbol{l})\gamma_5'$, $(\gamma_\mu-p_\mu/\boldsymbol{p}\boldsymbol{k}\cdot\boldsymbol{k}\boldsymbol{\gamma})\gamma_5'$, $(i\boldsymbol{\gamma}\boldsymbol{k})(l_\mu-p_\mu/\boldsymbol{p}\boldsymbol{k}\cdot\boldsymbol{k}\boldsymbol{l})\gamma_5'$, and $(i\boldsymbol{\gamma}\boldsymbol{k})\gamma_\mu\gamma_5'$, though c's would have different forms according to the method of calculation.

It is to be noted that the same arguments hold for the reversed process, that is, the matrix element for the radiative absorption of a spinless meson by a nucleon can be also expressed by four independent gauge invariant terms.

2. *The production of spin 1 mesons by photons*

For this process, (14) and (15) are to be replaced by

$$M=\bar{\psi}(\boldsymbol{p}')\varphi_\lambda(\boldsymbol{l})R_{\lambda\mu}(\boldsymbol{k},\boldsymbol{l},\boldsymbol{p},\boldsymbol{p}',\boldsymbol{\gamma})\psi(\boldsymbol{p})A_\mu(\boldsymbol{k}), \tag{17}$$

with

$$\begin{aligned}R_{\lambda\mu}(\boldsymbol{k},\boldsymbol{l},\boldsymbol{p},\boldsymbol{p}',\boldsymbol{\gamma})&=\gamma_5'G_{\mu\alpha}(\boldsymbol{k})R'_{\lambda\alpha}(\boldsymbol{k},\boldsymbol{l},\boldsymbol{p},\boldsymbol{p}',\boldsymbol{\gamma})\\&=\textstyle\sum_{l,m}c_{lm}(\Lambda_lG_{\mu\alpha}T_{\lambda\alpha m}\gamma_5').\end{aligned} \tag{18}$$

λ corresponding to the polarization of the produced meson. According to this additional degrees of freedom of $R_{\lambda\mu}$, though $N(\Lambda)$ is unaltered, $N(G_{\mu\alpha}T_{\lambda\alpha})$ becomes 7 in comparison with $N(G_{\mu\alpha}T_\alpha)=2$ in the preceding example: with the same $G_{\mu\alpha}$ as before and the Lorentz relation $l_\lambda\varphi_\lambda(\boldsymbol{l})=0$ for the meson, we must take $\gamma_\lambda\gamma_\alpha$, $\gamma_\alpha\gamma_\lambda$, $\gamma_\lambda l_\alpha$, $p_\lambda\gamma_\alpha$, $p_\lambda l_\alpha$, $k_\lambda\gamma_\alpha$, and $k_\lambda l_\alpha$ as the $T_{\lambda\alpha m}$'s. Therefore we have $2\times 7=14$ independent gauge invariant terms in this case**.

3. *The scattering of γ-rays by a Dirac particle (a charged or neutral spin 1/2 particle)*

Here we have the following expansion:

$$M=\bar{\psi}(\boldsymbol{p}')A_\nu(\boldsymbol{k}')R_{\mu\nu}(\boldsymbol{k},\boldsymbol{k}',\boldsymbol{p},\boldsymbol{p}',\boldsymbol{\gamma})A_\mu(\boldsymbol{k})\psi(\boldsymbol{p}), \tag{19}$$

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* In (K.K.N.) another set of four fundamental gauge invariant terms has been taken, the equivalence of both sets being easily proved.

** Among the 15 gauge invariant terms given by (7·6)~(7·10) on p. 888 of (K.K.N.), one of them can evidently be expressed in terms of the others.

with

$$R_{\mu\nu}(\boldsymbol{k}, \boldsymbol{k}', \boldsymbol{p}, \boldsymbol{p}', \gamma) = G_{\mu\alpha}(\boldsymbol{k})\, G_{\nu\beta}(\boldsymbol{k}')\, R_{\alpha\beta}(\boldsymbol{k}, \boldsymbol{k}', \boldsymbol{p}, \boldsymbol{p}', \gamma)$$
$$= \sum_{l,m} c_{lm} (\Lambda_l\, G_{\mu\alpha}\, G'_{\nu\beta}\, T_{\alpha\beta m}). \tag{20}$$

$N(\Lambda)$ is still 2. With the convenient choices of $G_{\mu\alpha}(\boldsymbol{k}) = (\delta_{\mu\alpha} + i\not{p}/\boldsymbol{pk} \cdot i\not{k}_\alpha)$ and $G_{\nu\beta}(\boldsymbol{k}') = (\delta_{\nu\beta} + i\not{p}_\nu/\boldsymbol{pk}' \cdot i\not{k}'_\beta)$, we can enumerate all possible independent $T_{\alpha\beta m}$'s, for example, $\gamma_\alpha\gamma_\beta$, $\gamma_\beta\gamma_\alpha$, $\gamma_\alpha\not{k}_\beta$, $\not{k}'_\alpha\gamma_\beta$, and $\not{k}'_\alpha\not{k}_\beta$, so that $N(G_{\mu\alpha}\, G'_{\nu\beta}\, T_{\alpha\beta}) = 5$. Thus it can be said that $2 \times 5 = 10$ independent gauge invariant terms are sufficient to expand any matrix element for the Compton scattering into gauge invariant form.

§ 4. Absolute selection rules for meson decay

An interesting consequence of the gauge invariant expansion theorem is that it can give some absolute selection rules for meson decay. In fact, if the photons are involved in the decay products, the G-factor might diminish the number of characteristic terms to zero. In such cases, any gauge invariant expression cannot be constructed from available four-momenta and so the decay process are forbidden. Various absolute selection rules for meson decay have been already derived from the general principle of invariance under space rotation and inversion[3]. In these derivations the gauge invariance is of course taken into consideration but in the sense that the photon has only two independent polarizations. Since the gauge invariant expansion theorem is based on the Lorentz covariance, our attempt to derive the absolute selection rules is essentially the same as the previous ones. As might be expected, our theorem, too, is effective for this purpose only when the number of participating particles is small. For many particle decays one cannot say anything definite about the selection rules without sufficient informations on the details of expansion coefficient, as will be seen in the second example below. This corresponds to the circumstance in the previous considerations that the asymmetry of the final state make it possible to find the absolute selection rules.

1. A meson of spin 0 cannot decay into a photon and a spin 0 meson

The matrix element for this decay process is in general expressed in a form:

$$M = A_\mu(\boldsymbol{k})\, \varphi(\boldsymbol{l})\, R_\mu(\boldsymbol{k}, \boldsymbol{l})\, \varphi'(\boldsymbol{k} + \boldsymbol{l}), \tag{21}$$

where $R_\mu(\boldsymbol{k}, \boldsymbol{l})$ behaves as a vector or pseudovector according as the decaying and decayed mesons have the same or opposite parity.

In the former case, combined with the G-factor for $A_\mu(\boldsymbol{k})$, $R_\mu(\boldsymbol{k}, \boldsymbol{l})$ can be expanded as*

$$R_\mu(\boldsymbol{k}, \boldsymbol{l}) = G_{\mu\alpha}(\boldsymbol{k})\, R_\alpha(\boldsymbol{k}, \boldsymbol{l}) = \sum_m c_m (G_{\mu\alpha}\, T_{\alpha m})$$
$$= G_{\mu\alpha}(\boldsymbol{k})\, (c_1\, k_\alpha + c_2\, l_\alpha). \tag{22}$$

With $G_{\mu\alpha}(\boldsymbol{k}) = (\delta_{\mu\alpha} - l_\mu/\boldsymbol{kl} \cdot k_\alpha)$, we have $G_{\mu\alpha} k_\alpha = 0$ and $G_{\mu\alpha} l_\alpha = 0$ which imply $N(G_{\mu\alpha}\, T_\alpha) = 0$.

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* Since R in this section does not contain γ-matrices and we have $\Lambda_1 = 1$ alone, we omit Λ_l and write c_m instead of c_{1m} in the expansion.

In the latter case, the selection rule is evident because it needs at least three linearly independent four-vectors in order to construct the pseudovector $R_\mu(\boldsymbol{k}, \boldsymbol{l})$ whereas we have only two available four-vectors $\boldsymbol{k}$ and $\boldsymbol{l}$.

2. *A neutral meson of spin 1 cannot decay into two photons*

The matrix element for the process is given by

$$M = A_\mu(\boldsymbol{k})\, A_\nu(\boldsymbol{k}')\, R_{\lambda\mu\nu}(\boldsymbol{k}, \boldsymbol{k}')\, \varphi_\lambda(\boldsymbol{k}+\boldsymbol{k}'), \tag{23}$$

where $\boldsymbol{k}$, $\boldsymbol{k}'$ are the four-momenta of the decay photons and satisfy $(\boldsymbol{k}+\boldsymbol{k}')^2 = -\boldsymbol{\varkappa}^2$, $\boldsymbol{\varkappa}$ being the mass of the decaying meson. $R_{\lambda\mu\nu}$ has the transformation property as a tensor of third rank or its dual according as a meson is vector or pseudovector. Ignoring the cumbersome non-gauge-invariant ambiguity, though it might appear, the gauge invariance of the matrix element permits the introduction of two G-factors for $A_\mu(\boldsymbol{k})$ and $A_\nu(\boldsymbol{k}')$ to develop $R_{\lambda\mu\nu}(\boldsymbol{k}, \boldsymbol{k}')$. It is to be noted that the expansion coefficients in this case are the functions of $\boldsymbol{\varkappa}^2$ and dependent on neither $\boldsymbol{k}$ nor $\boldsymbol{k}'$, because the only available scalar product of the external four-momenta is $(\boldsymbol{k}\boldsymbol{k}')$ which is equal to $-\boldsymbol{\varkappa}^2/2$.

(a) Neutral vector meson

If we choose $\boldsymbol{f} = \boldsymbol{k}'$, $\boldsymbol{f}' = \boldsymbol{k}$ as two arbitrary functions, $R_{\lambda\mu\nu}$ is reduced to

$$\begin{aligned} R_{\lambda\mu\nu}(\boldsymbol{k}, \boldsymbol{k}') &= G_{\mu\alpha}(\boldsymbol{k})\, G_{\nu\beta}(\boldsymbol{k}')\, R_{\lambda\alpha\beta}(\boldsymbol{k}, \boldsymbol{k}') \\ &= G_{\mu\alpha}(\boldsymbol{k})\, G_{\nu\beta}(\boldsymbol{k}')\, (c_1\, k_\lambda + c_2\, k'_\lambda)\, \delta_{\alpha\beta}, \end{aligned} \tag{24}$$

because of $G_{\mu\alpha} k_\alpha = G_{\mu\alpha} k'_\alpha = G'_{\nu\beta} k_\beta = G'_{\nu\beta} k'_\beta = 0$. But, as the matrix element is symmetrical with respect to two photons, i.e., $R_{\lambda\mu\nu}(\boldsymbol{k}, \boldsymbol{k}') = R_{\lambda\nu\mu}(\boldsymbol{k}', \boldsymbol{k})$, and c_1, c_2 are the function of $\boldsymbol{\varkappa}^2$ only, (24) is equal to

$$(1/2)\, G_{\mu\alpha} G'_{\nu\beta} (c_1 + c_2)\, (\boldsymbol{k}+\boldsymbol{k}')_\lambda \delta_{\alpha\beta},$$

which vanishes in virtue of the relation $(\boldsymbol{k}+\boldsymbol{k}')_\lambda \varphi_\lambda(\boldsymbol{k}+\boldsymbol{k}') = 0$.

(b) Neutral pseudovector meson

It is most convenient to employ a wholly antisymmetric unit tensor $\varepsilon(\mu\nu\rho\sigma)$ to indicate the dual property of $R_{\lambda\mu\nu}$ in this case. With the same G-factors as (a) $R_{\lambda\mu\nu}$ can then be expanded into

$$\begin{aligned} R_{\lambda\mu\nu}(\boldsymbol{k}, \boldsymbol{k}') = G_{\mu\alpha}(\boldsymbol{k})\, G_{\nu\beta}(\boldsymbol{k}') [&c_1\, \varepsilon(\lambda\alpha\beta\rho)\, k_\rho + c_2\, \varepsilon(\lambda\alpha\beta\rho)\, k'_\rho \\ &+ c_3\, \varepsilon(\lambda\alpha\beta\rho)\, k_\rho k'_\sigma k_\lambda + c_4\, \varepsilon(\alpha\beta\rho\sigma)\, k_\rho k'_\sigma k'_\lambda], \end{aligned} \tag{25}$$

which is reduced, by the above symmetry argument, to

$$= (1/2)\, G_{\mu\alpha} G'_{\nu\beta} [(c_1 + c_2)\, \varepsilon(\lambda\alpha\beta\rho)\, (k-k')_\rho + (c_3 + c_4)\, \varepsilon(\alpha\beta\rho\sigma)\, k'_\rho k_\sigma (k+k')_\lambda],$$

where the latter term becomes zero, but the former affords us a gauge invariant term of the form

$$-(1/\boldsymbol{\varkappa}^2)\, (c_1 + c_2) \{ (\boldsymbol{k}\boldsymbol{k}')\, \varepsilon(\lambda\mu\nu\rho)\, (k-k')_\rho - k'_\mu \varepsilon(\lambda\nu\rho\sigma)\, k_\rho k'_\sigma + k_\nu \varepsilon(\lambda\mu\rho\sigma)\, k_\rho k'_\sigma \}. \tag{26}$$

However, taking account of A_μ, A'_ν and φ_λ, this changes into*

$$-(1/\kappa^2)(c_1+c_2)(k+k')_\lambda \varepsilon(\mu\nu\rho\sigma) k_\rho k'_\sigma,$$

which again vanishes.

Thus, with but a little information on the expansion coefficients c_m's, we can rule out absolutely the decay of a neutral meson with spin 1 into two photons.

§ 5. Concluding remarks

We have studied the general feature of the matrix elements for the transition concerning photons or external electromagnetic fields when only the composition of the particles or fields in the initial and final states of transition is given but the mode of coupling between them is not known. The introduction of G-factors has made it possible to transform the matrix elements into obviously gauge invariant forms. Moreover, by combining the G-factors with the general expansion theorem which is based on the Lorentz covariance, we have been able to show that any matrix element can be expanded in terms of a definite number of independent gauge invariant terms characteristic of the given process.

We wish finally to comment upon the significance of our procedure. Firstly, a particular emphasis should be placed on the fact that the subject of our considerations is not the inner structure but the superficial feature of a transition. As a result, our method of analysis is effective to all present as well as future problems so long as they satisfy the requirement of gauge invariance. For example, the inclusion of nucleon isobars in intermediate states, the consistent formulation of extended source or interaction, and so on, would require no alteration of our analysis.

Secondly, the gauge invariant terms themselves represent all possible gauge invariant interactions between two given states, so that they may possibly correspond to some physical realities. Thus the interpretation of these terms will help the analysis of the results obtained by the calculation, as was done by Koba et al. in the $\gamma-\pi$ production where four independent terms are interpreted as the interaction of the photon with the current, with the magnetic moment of the nucleon before and after the meson emission, and the virtual spin effect, and will make easy the introduction of phenomenological interactions to bring the theoretical predictions to better agreement with the experimental results.

In conclusion we should like to express our cordial thanks to Messrs. S. Hayakawa and K. Nishijima for their invaluable discussions, especially on the absolute selection rules for meson decays. One of us (M.K.) is indebted to the Yukawa Yomiuri Fellowship for the financial aid.

References

1) Z. Koba, T. Kotani and S. Nakai, Prog. Theor. Phys. **6** (1951), 849.
S. Minami, Prog. Theor. Phys. **7** (1952), 69.
2) Z. Koba, N. Mugibayashi and S. Nakai, Prog. Theor. Phys. **6** (1951), 322.
3) C. N. Yang, Phys. Rev. **77** (1950); 242.
D. C. Peaslee, Helv. Phys. Acta **23** (1950), 845; **24** (1951), 298.

* Compare, p. 336 of reference 2.

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Slow Neutrons in the Cosmic Radiation, I

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The diffusion of cosmic-ray neutrons in the atmosphere is calculated by using recent experimental value on neutron cross sections for the computation of the age τ. It is found that the correct boundary condition at the top of the atmosphere is necessary for the analysis of the data at stratosphere. Assuming the neutron sources to be stars, the altitude variation and the absolute density of slow neutrons is obtained and compared with experiments.

§ 1. Introduction

In last several years, detailed investigations on neutron component were performed by various authors. They showed that the density of slow neutrons increases exponentially with decreasing atmospheric depth, and has a flat maximum near 100 g/cm^2. This altitude variation is very similar to that of cosmic ray stars. One may thus infer that the neutrons are of secondary origin and produced in stars by N-component. Bethe, Korff and Placzek gave an extensive theoretical analysis[1] which satisfactorily explains experimental data. A comprehensive survey of earlier experimental works and theoretical extension were given by Flügge[2].

Although the qualitative behavior of cosmic ray neutrons, i.e. its diffusion, slowing down and capture by nitrogen atom, can be understood through these works, recent advancement made in this field seems to require more exact calculations which are facilitated by precise measurements on neutron cross section covering a wide range of energies.

Refined calculations on the neutron component seem to us worth while on two purposes. One is concerned with the primary radiation and the other with the nucleon cascade of the N-component.

As for the former we must remark that the neutron component has the largest latitude effect among all others. Thus it can be a good indicator for the primary radiations of such low energies as to be influenced by the terrestrial magnetic field.

Application to the nucleon cascade can easily be seen from the fact that evaporated neutrons are produced in every nuclear event even if its energy is not high enough to produce a visible track in the photographic emulsion. That is, neutrons can be used as an energy-insensitive detector for nuclear interactions, in contrast to associated penetrating showers or stars.

Unfortunately calculations can be performed in a closed way only for the slowing down process of slow neutrons by their elastic collisions with nuclei. We have no reliable method for neutrons in higher energy region where inelastic collisions or other nuclear

transmutations take an important part. Therefore in this paper, we confine ourselves to slow neutrons that the age theory of Fermi is applicable. Revised value of age parameter τ is computed, referring to the recently published value for neutron cross section. The boundary condition at the top of atmosphere is examined which has heretofore been put simply to zero. These revisions are most significant for the interpretation on high altitude measurements.

§ 2. Age equation

(*1*) *Age parameter* Following Fermi's theory of neutron slowing down, the age parameter τ is defined as,

$$\tau=\int_0^u l^2(u)\,du/3\xi(1-<\cos\theta>_{AV}), \qquad u=\ln(E_0/E), \tag{1}$$

where E_0 and E are an initial energy and the energy of the neutron slowed down, respectively. ξ, the average logarithmic energy loss per collision, is

$$\xi=2/A_{\text{eff}}\approx 0.141,$$

where A_{eff} is the effective mass number of air nuclei, 14.6. $<\cos\theta>_{AV}$, the mean scattering angle in laboratory system, is estimated as,

$$<\cos\theta>_{AV}\approx 2/3A_{\text{eff}}=0.046.$$

$l(u)$ is the scattering mean free path of neutrons with energy E.

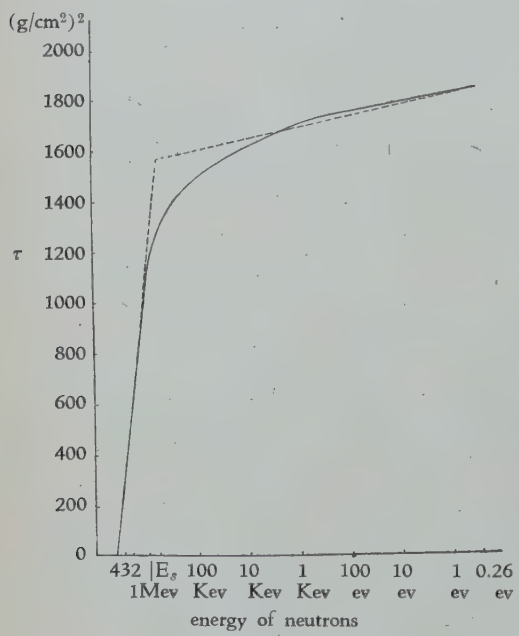

Fig. 1. Relation between energy and age. Full line is obtained by numerical integration, and dashed line by assuming two constant mean free paths.

In the previous treatment of Bethe, Korff and Placzek[1] and Flügge[2], $l(u)$ was assumed as constant and equal to 18g/cm² or 2.6g/cm² above or below E_s, the numerical value of E_s being taken as 10 Kev or 100 Kev. Here we take the latest experimental value of $l(u)$[3] and integrate (1) numerically. This result is shown in Fig. 1. In accordance with Davis[4], we assume that all neutrons are captured at $E_c=0.26$ev.

The lowest excited states of N^{14} and O^{16} nucleus is known to be at 2.3 Mev and 6.05 Mev, respectively. Thus the neutrons of energy above 2.3 Mev can be scattered inelastically by nitrogen nuclei. By a detailed study which will be shown in a following paper[5], we can show that the slowing down processes by elastic collisions dominate in the energy region below ~4Mev, and inelastic ones, (n,p) and (n,α) reactions compete at higher energy.

(2) *Diffusion equation* We shall first calculate the Green function $\chi(\tau, z, z')$ for the age equation, i.e. the solution with a monochromatic plane neutron source at an atomospheric depth z',

$$\frac{\partial}{\partial\tau}\chi(\tau, z, z') = \frac{\partial^2}{\partial z^2}\chi(\tau, z\, z'), \tag{2}$$

under an initial condition,

$$\chi = \delta(z - z'), \quad \text{at} \quad \tau = 0,$$

and boundary conditions,

$$\chi(\tau, z, z') \to 0, \qquad \text{as} \quad z \to \infty, \quad \text{for all } \tau, \tag{2a}$$

$$\chi(\tau, z, z') = \frac{2}{3}\cdot\frac{l(u)}{1 - <\cos\theta>_{AV}}\cdot\frac{\partial\chi(\tau, z, z')}{\partial z}, \quad \text{at} \quad z = 0, \quad \text{for all } \tau. \tag{2b}$$

The condition (2b) follows from that the total incoming flux of neutrons should be zero at the top of the atmosphere.

Except near the top of the atmosphere, an approximate solution can be obtained by the simple boundary condition,

$$\chi(\tau, z, z') = 0, \quad \text{at} \quad z = 0, \quad \text{for all } \tau.$$

This approximation was used by Flügge[2], Davis[4] and others. Then the equation does not explicitly contain the mean free path $l(u)$, and is dependent only on the age parameter τ. Its solution will hereafter be denoted by χ_0 and is given by,

$$\chi_0(\tau, z, z') = \frac{1}{\sqrt{2\pi\tau}}\left[\exp\left(-\frac{(z - z')^2}{4\tau}\right) - \exp\left(-\frac{(z + z')^2}{4\tau}\right)\right]. \tag{3}$$

The exact solution of (1) with (2b) can not in general be obtained analytically. In the case of a constant mean free path, Marshak[6] gave the following solution,

$$\chi(\tau, z, z') = \frac{1}{\sqrt{2\pi\tau}}\left[\exp\left(-\frac{(z + z')^2}{4\tau}\right) + \exp\left(-\frac{(z - z')^2}{4\tau}\right)\right.$$
$$\left. - A\exp(A\tau^2 + A(z + z'))\left(1 - \Phi\left(A\sqrt{\tau} + \frac{(z + z')}{2\sqrt{\tau}}\right)\right)\right], \tag{4}$$

where

$$A = 3/2\,\bar{l},$$

and

$$\bar{l} = l/(1 - <\cos\theta>_{AV}),$$

and $\Phi(x)$ is the Gaussian integral. In practical cases, $A^2\tau$ is much larger than one, and Gaussian integral is well approximated by its asymptotic form. Then we obtain,

$$\chi = \frac{1}{\sqrt{2\pi\tau}}\left[\exp\left(-\frac{(z - z')^2}{4\tau}\right) - \left(\frac{2A\tau - z - z'}{2A\tau - z + z'}\right)\exp\left(-\frac{(z + z')^2}{4\tau}\right)\right], \tag{5}$$

or

$$\chi = \chi_0 + \delta\chi,$$

$$\delta\chi = \frac{1}{\sqrt{\pi\tau}} \frac{z+z'}{2A\tau+z+z'} \exp\left(-\frac{(z+z')^2}{4\tau}\right). \tag{6}$$

(3) *Validity of approximations* When both z and z' are much larger than $\sqrt{\tau}$, χ can be well approximated by the first term of χ_0,

$$\chi \sim \frac{1}{\sqrt{2\pi\tau}} \exp\left(-\frac{(z-z')^2}{4\tau}\right). \tag{7}$$

At depth smaller than $2\sqrt{\tau}$, no approximation is permitted and the correct setting of boundary condition is necessitated. To see the behavior of solutions, we calculate χ and χ_0 for several values of z and z', and show them in Fig. 2. Here we take $l/\sqrt{\tau}=0.45$.

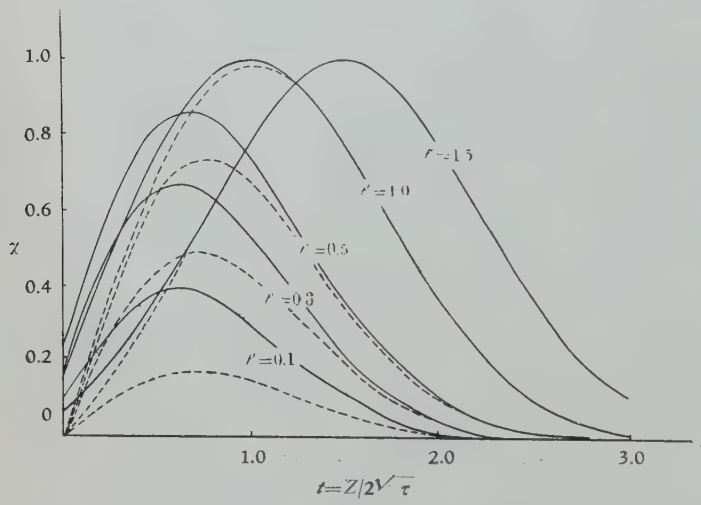

Fig. 2. Density distribution for plane sources at various altitudes, t'. t and t' are atmospheric depths measured in unit of $2\sqrt{\tau}$. Full line is with correction and dashed line is without correction.

In practical case for air nuclei, the mean free path l can be approximated by two constant values, i.e. 18 g/cm^2 and 2.8 g/cm^2 for higher and lower energies than E_s, respectively, E_s being 0.57 Mev. The above value of $l/\sqrt{\tau}=0.45$ corresponds to $l=18$ g/cm^2 and $\tau=1570\,(\mathrm{g/cm^2})^2$, which is the age from 4 Mev to E_s. Therefore χ represents the density distribution of neutrons with energy E_s diffused from the plane source of 4 Mev neutrons.

The age from E_s to 0.26 ev, the mean energy for capture by N^{14}, is $280\,(\mathrm{g/cm^2})^2$, and it is much smaller than the age from 4 Mev to E_s. Therefore we can suppose that the density distribution of slow neutrons does not differ greatly from the above obtained χ except for $z \leq 280$ g/cm^2. Comparison of χ with χ_0 shows the necessity of the correct setting of the boundary condition for the analysis of slow neutrons at the upper stratosphere.

(4) *Reciprocity* From the symmetry of Green function $\chi(z, z')$ on z and z', we can have another interpretation of χ. That is $\chi(z, z')$ gives the contribution rate of source at z on the slow neutron density at z'. When we measure the slow neutrons at stratosphere, we find from Fig. 2 that most part of them come from the sources at $z \sim \sqrt{\tau}$. Therefore many neutrons which are produced at smaller depths $< \sqrt{\tau}$, turn out to escape out the atmosphere during the slowing down processes.

§ 3. Altitude variation

At greater atmospheric depths $z \ll \sqrt{\tau}$, the altitude variation of slow neutrons will be completely determined by the distribution of neutron sources. On the other hand, in the stratosphere we can suppose from the preceding discussions that it greatly depends on the diffusion process, and not so much on the source function. To see these facts more clearly, we shall calculate the altitude variation of slow neutrons for a certain source function $S(z')$.

As the main part of neutron sources can be considered to be nuclear disintegrations observed as stars, we have taken the form of source function $S(z')$ as to represent well the altitude variation of stars.

$$S(z') = \begin{cases} J_0 \exp(-a/\lambda), & \text{for} \quad z' < a, \\ J_0 \exp(-z'/\lambda), & \text{for} \quad z' > a. \end{cases} \tag{8}$$

For example, $S(z')$ with $a = 100$ g/cm^2 and $\lambda = 140$ g/cm^2 reproduce fairly well the experimental curve of photographic work of Lord[7]. Now the neutron density $\Psi(z, \tau)$ can be given as follows,

$$\Psi(z, \tau) = \int dz' \chi(\tau, z, z') S(z'). \tag{9}$$

At greater depths $z \ll \sqrt{\tau}$, $\chi(\tau, z, z')$ can be approximated by χ_0 in (3). Thus we have for $z > a$,

$$\Psi(z, \tau) \approx \Psi_0(z, \tau) = \int dz' \chi_0(\tau, z, z') S(z')$$

$$= (J_0/2)\exp(-a/\lambda)[2\Phi(z/2\sqrt{\tau}) - \Phi((z-a)/2\sqrt{\tau}) - \Phi((z+a)/2\sqrt{\tau})]$$

$$+ (J_0/2)\exp(\tau/\lambda^2)\left[\exp(-z/\lambda)\left(1 + \Phi\left(\left(z - a - \frac{2\tau}{\lambda}\right)\Big/ 2\sqrt{\tau}\right)\right)\right.$$

$$\left. - \exp(z/\lambda)\left(1 - \Phi\left(\left(z + a + \frac{2\tau}{\lambda}\right)\Big/ 2\sqrt{\tau}\right)\right)\right]. \tag{10}$$

For larger z, Ψ_0 has an asymptotic form as,

$$\Psi_0(z, \tau) \approx J_0 \exp[(\tau/\lambda^2) - (z/\lambda)], \tag{11}$$

and it depends on z in the same way as the source function $S(z)$ through the factor $\exp(-z/\lambda)$.

Exact calculations are necessitated for smaller depths. In the approximation of constant mean free path, the Green function $\chi = \chi_0 + \delta\chi$ is given by (5). After the integration in (9), we have the following correction terms for the neutron density Ψ :

$$\Psi = \Psi_0 + \delta\Psi,$$

$$\delta\Psi = J_0 \exp(-a/\lambda) \frac{1}{\sqrt{\pi}} \left\{\left(1\Big/\left(A\sqrt{\tau} + \frac{z}{2\sqrt{\tau}}\right)\right)\exp(-z^2/4\tau)\right.$$

$$-\left(1\Big/\left(A\sqrt{\tau}+\frac{a+z}{2\sqrt{\tau}}\right)\right)\exp(-(z+a)^2/4\tau)\Big\}$$

$$+J_0\lambda A/(\lambda A-1)\left\{\exp(-a/\lambda)\,\frac{1}{\sqrt{\pi}}\cdot\frac{1}{A\sqrt{\tau}+(a+z)/2\sqrt{\tau}}\exp[-(z+a)^2/4\tau]\right\}$$

$$-J_0\frac{1}{\lambda A-1}\exp(\tau/\lambda^2)\exp(z/\lambda)\left(1-\Phi\left(\left(a+z+\frac{2\tau}{\lambda}\right)\Big/2\sqrt{\tau}\right)\right). \qquad (12)$$

As was shown in § 2 (3), this approximation can be valid down to energy E_s. Applying the numerical values, $l=18$ g/cm^2 and $\tau=1570$ (g/cm^2)^2, we have the density of neutrons of this energy E_s. Fig. 3 shows the results for $a=0$ and 100 g/cm^2. We can see

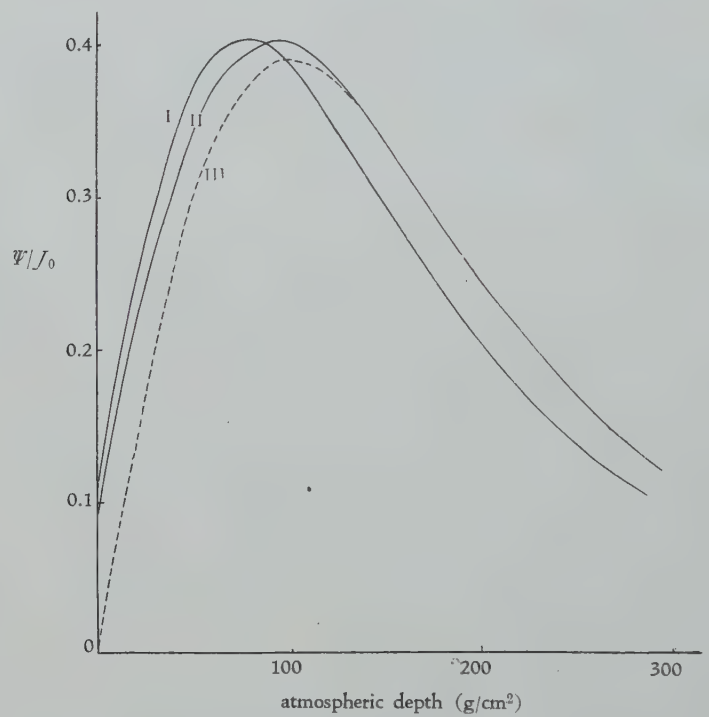

Fig. 3. Density distribution at $E=E_s$. I; $a=0$, with correction. II; $a=100$ g/cm^2, with correction. III; $a=100$ g/cm^2, without correction.

that the altitude variation does not depend sensitively on the value of a as was expected. In the following calculation, we take $a=100$ g/cm^2, throughout.

To calculate the density of slower neutrons, we must solve further diffusion processes down to $E_c=0.26$ ev. From E_s to E_0 the age is 280 (g/cm^2)^2 and the mean free path can be approximated by a constant, 2.8 g/cm^2. Except near the very top of atmosphere, $z<\sqrt{280}$, χ can again be replaced by χ_0. In the case of very small depth we use the Green function with constant mean free path.

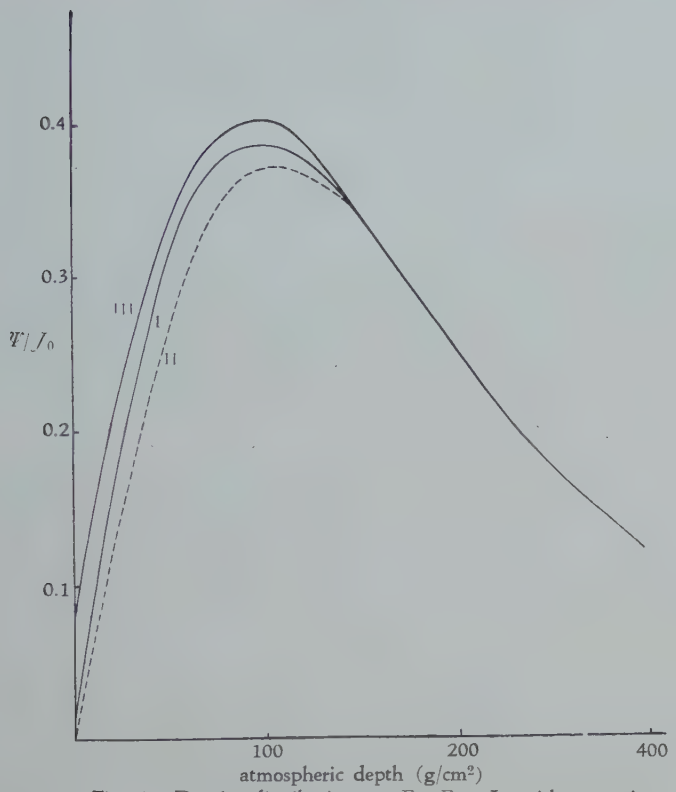

Fig. 4. Density distribution at $E=E_0$. I; with correction. II; without correction.
III; reproduction of curve II of Fig. 3.

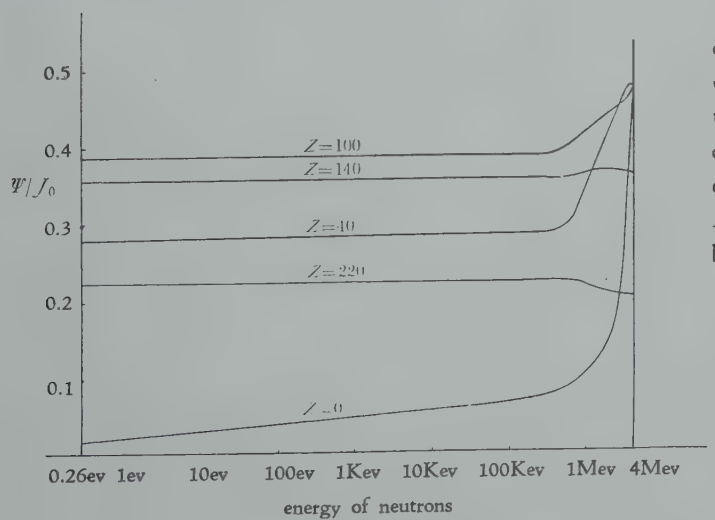

Fig. 5. Slowing down density of neutrons. Parameter the depth in g/cm². Z must be read as z.

We can now obtain the complete altitude variation of slow neutrons combining this with the previous result as source function, and show the result in Fig. 4. The τ-spectrum of neutrons is also obtained at a given depth by varying τ in $\Psi(z,\tau)$ which was calculated above. This result is shown in Fig. 5. The spectrum at 220 g/cm² is almost flat and it shows that the equilibrium between production and absorption is already reached at this depth. At smaller depths, the rate of high energy component becomes larger compared to low energy ones. This is due to the fact that some neutrons escape out in the course of slowing down processes.

$\Psi(z,\ \tau)$ is currently called as slowing down density. The energy spectrum $\Phi(z,\ E)dE$, i.e. the density of neutrons with energy between E and $E+dE$ is related to $\Psi(z,\tau)$ by the following formula,

$$\Phi(z,\ E)dE=\Psi(z,\ \tau)\times\frac{l}{v\xi}\cdot\frac{dE}{E}.$$

§ 4. Comparison with experiments

We have seen from previous calculations that the elastic collisions in energy region $4 \sim 0.5$ Mev are most predominant for diffusion processes of neutrons. But unfortunately we have little knowledge on the energy spectrum of neutron sources, and thus we are hard to obtain an accurate estimation for the age τ. On these neutron sources, we shall discuss in a separate paper together with the inelastic collisions and other nuclear transmutations. Here we shall discuss the altitude variation and absolute rate of the slow neutron density under the assumption of monochromatic source of 4 Mev. Comparison of the experimental with calculated values will give us some information on the above question. The source energy 4 Mev is taken because, as was shown earlier, it seems to be an upper limit for the applicability of the age theory.

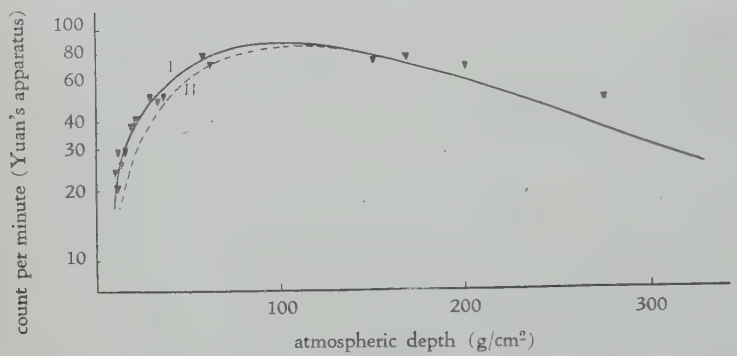

Fig. 6. Theoretical and experimental altitude dependence. I; theoretical with correction. II; theoretical without correction. ▽; Yuan's experiment.

(1) *Comparison with experiments of Cd-difference* In Fig. 6, we reproduce the experimental value of Yuan[8] taken by Cd-difference. This can be compared directly with the slow neutron density $\Psi(z, \tau)$ which was calculated in the previous section and is shown as curve I in the same figure. The maximum of our curve I occurs near to 110 g/cm^2 in accordance with the experimental value of Yuan, 114 g/cm^2. From this agreement we see that our simplified model can give good estimation for the age τ.

Curve II is obtained by the approximate solution Ψ_0 with zero boundary condition. The difference between I and II shows the importance of the correct boundary condition for the analysis of data taken at stratosphere.

The deviation at depths greater than 200 g/cm^2 is perhaps due to the difference between our assumption of $\lambda = 140$ g/cm^2 and the absorption mean free path 156 g/cm^2 of slow neutrons obtained by Yuan. If we took ~ 155 g/cm^2 for λ, a complete agreement could be obtained, and the experimental value of λ for stars and slow neutrons may have this order of uncertainty. As we are intending mainly to discuss the altitude dependence at higher altitudes, we will not discuss this point any further.

(2) *Comparison with experiments of enriched and natural BF_3 difference* For the case of $1/v$ detector of this type, some cares must be taken for the change of energy spectrum of neutrons. The counting rate at depth z is proportional to

$$\int dE \Psi(z, E) \frac{\tau'}{l_{abs.}},$$

where v is the velocity, and $l_{abs.}$ is the absorption mean free path for B^{10}. $\Phi(z, E)$ is the neutron density with energy between E and $E+dE$, and it can be expressed by the slowing down density $\Psi(z, \tau)$ as was shown in § 3. Then we have for the counting rate,

$$\int \frac{dE}{E} \Psi(z, \tau) \frac{l}{v\xi} \cdot \frac{v}{l_{abs.}} \propto \int \Psi(z, \tau) \frac{dE}{E^{3/2}} .$$

We have already calculated $\Psi(z, \tau)$ at several depths in § 3. Performing the integration numerically, the effect of change in energy spectrum can be estimated. It increases with decreasing depth, but amounts to only little even at smaller depths, as is shown in Fig. 7.

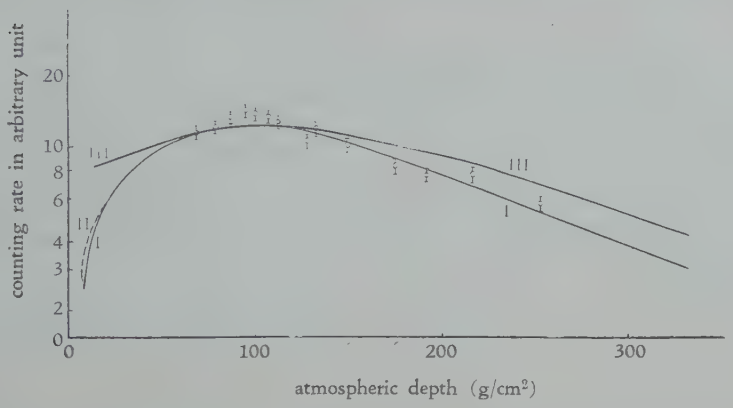

Fig. 7. Comparison with experiments of 1/v detector. I; theoretical altitude dependence for Cd difference; reproduction of curve I of Fig. 6. II; theoretical altitude dependence for enriched and natural BF_3 difference. III; Staker's experiment. Φ; Davis' experiment. (experimental values are normalized to the theoretical curves at the maximum).

The experiments of Staker et al.[9] and Davis[4] are of this type and their results are shown in Fig. 7, together with the calculated ones. The result of the latter author agrees well with the theoretical one, though it is limited to depths below 80 g/cm². On the other hand, Staker's value is much larger at small depths. It seems hard to give a theoretical account for this deviation, though his experiment was carried out at lower latitude, 30° N.

(3) *Absolute counting rate* Now we investigate the relation between the rates of slow neutron capture and of star production. According to Lord[7], the production rate of stars with two or more prongs is about 2300 per day per c.c. of emulsion at atmospheric depth 100 g/cm² and geomagnetic latitude 50° N. As this figure includes stars of light as well as heavy nuclei in emulsion, we convert it to the star rate per gram of gelatine assuming the geometrical nuclear cross section. From this we can estimate the star production in air at this altitude as 0.69 per gram per minute.

If we assume that n neutrons of 4 Mev are produced in every stars on an average, we can obtain the source function. This is given by (8) with $a=100$ g/cm², $\lambda=140$ g/cm² and $J_0=1.41$ n per gram of air per minute. We can readily obtain the absolute density at various altitudes by inserting the above values in preceding calculations.

Many experimental workers gave the absolute slow neutron absorption rate in air per unit time and mass. This should be directly compared with slowing down density $\Psi(z, \tau)$ at the age τ_c. At the maximum of altitude variation, $z=114$ g/cm², we have

$$\Psi(114\ \mathrm{g/cm^2},\ \tau_e) = 0.550\ n/\mathrm{gram\ of\ air,\ min.}$$

At this altitude, Yuan[8] gave 1.37 per gram of air per minute. Comparing between these two values, we have,

$$n = 1.37/0.55 = 2.50.$$

At the same latitude, the experiments of Davis[4] and Korff and Hamermesh[10] gave about half the value given by Yuan[8], though the correction remarked by Lattimore[11] is made. On the other hand Simpson[12] gave, for the integrated capture rate, 8 per cm^2 column of atmosphere per second. The corresponding rate of Yuan is 7.1. This agreement and the reasonable value $n = 2.5$ will support the absolute rate of Yuan.

§ 5. Concluding remarks

We have analysed the slow neutrons in the atmosphere, and obtained altitude variation which agrees well with experimental data of Yuan. From comparison of absolute density we have the neutron multiplicity $n \approx 2$ per star. These facts will show that our model on neutron sources gives a good estimate on the age τ, in spite of its rather simplified form of monochromatic sources.

Thus, we can apply this model for the discussion of other problems concerning slow neutrons, such as latitude effect, time variations and so on. These analysis will be given in a following paper[5].

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References

1) H. A. Bethe, S. A. Korff and G. Placzek, Phys. Rev. **57** (1940), 573.
2) S. Flügge, Cosmic Radiation, Dover Publication, ed. by Heisenberg, (1946), *Chap.* XIV
3) R. K. Adair, Rev. Mod. Phys. **22** (1950), 849.
4) W. O. Davis, Phys. Rev. **80** (1950), 150.
5) Y. Fujimoto and T. Tamura, to be published.
6) R. E. Marshak, Rev. Mod. Phys. **19** (1947), 185.
7) J. J. Lord, Phys. Rev. **81** (1951), 901.
8) L. C. L. Yuan, Phys. Rev. **81** (1951), 175.
9) W. P. Staker, Phys. Rev. **80** (1950), 52 and 150.
W. P. Staker, M. Pacalow and S. A. Korff, Phys. Rev. **81** (1951), 889.
10) S. A. Korff and B. Hamermesh, Phys. Rev. **69** (1946), 185.
11) S. Lattimore, Phys. Rev. **81** (1951), 643.
12) J. A. Simpson, Phys. Rev. **83** (1951), 1175.

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Theory of the Nuclear Magnetic Relaxation in Crystalline Solids, I

—— *Direct Process* ——

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As is well-known, the nuclear magnetic relaxation due to the lattice vibrations of the crystalline solids has not yet been completely clarified since both theories proposed by Bloembergen and Pound seem to be valid for the special kinds of crystalline solids. In view of these situations, therefore, we have here presented theoretically a new mechanism of the nuclear magnetic relaxation in crystalline solids in which the crystal electron plays an important role in the intermediate states of the second or third order transition processes. Such a mechanism for the nuclear magnetic relaxation may be considered to be actually realized in all the crystalline solids. The orders of magnitude for the nuclear magnetic relaxation times are found to be in good agreements with the available experimental observations in view of our general theory being based upon the rather simplified model of Wilson for the crystalline insulators.

§ 1. Introduction

It is well-recognized that the direct coupling between the nuclear spin and the crystal-lattice vibrations, through the magnetic dipolar interactions of the nuclei, fails completely to account for the relaxation times commonly observed in crystals at low and room temperatures. In fact the times of the nuclear spin-lattice relaxations in solids appear to range between about 10^{-4} and 10^{2} seconds according to the available experimental observations,[1] while, Waller's theory[2] based upon the magnetic dipolar interactions of the nuclei has yielded extraordinary large relaxation times, for example, 10^{10} seconds or more, at room temperatures, for F^{19} nucleus in CaF_2 in contradistinction to the measured values of a few seconds. On the other hand, according to Bloembergen, Purcell, Pound and others,[3] the measured relaxation times in liquids and certain kinds of solids appear at least qualitatively to be interpreted through the nuclear magnetic dipolar interactions although, in the mentioned substances, rotating or jumping constituent-nuclei or complex groups in solids and Brownian motions of molecules in liquids have resulted in shortened relaxation times. In the above mentioned substances, therefore, the average displacements in the thermal motions of nuclei responsible for the nuclear magnetic absorption seem to be quite large compared with those of the thermal vibrations of crystal lattice, which leads to the relatively large coupling between the nuclear spin system and the thermal motion of the former class of substances, i. e., the shorter relaxation times in accordance with the experimental observations. Furthermore, in the metallic crystal, the situation is a little different[4] from the

other kinds of crystals, in which the relatively large magnetic dipolar interactions between the nuclei and the conduction electrons near the Fermi energy have resulted in shortening the mentioned relaxation time in accordance with Bloembergen's experimental observation[3] in metallic copper.

In view of these situations, Bloembergen[6] has recently proposed the so-called spin diffusion theory in which some kind of paramagnetic impurity atoms, contained in crystals naturally or artificially, may take an essential role of greatly shortening the relaxation times of the non-metallic crystals, and, on the other hand, Pound[7] has stressed the fact that the electrical interactions of the electric quadrupole moments within nuclei with the nearby charge distribution within the crystal have actually shortened the nuclear relaxation times.

Now, although the mentioned mechanisms, due to Bloembergen or Pound, for the nuclear spin-lattice relaxation are actually valid for certain kinds of crystals, still those are not considered to be most commonly realized in almost all the crystals which have been observed so far. We, therefore, shall present here a new mechanism for the nuclear spin-lattice relaxation in crystals, in which the magnetic dipolar interactions between the nuclei and the crystal electrons in filled band, and the electrical coupling between the crystal electrons and the lattice vibrations take essential parts simultaneously in the nuclear spin-lattice relaxation processes, and, further, the transitions of the crystal electrons are taken place in the intermediate states alone, being called the virtual transitions. Similarly to Waller's theory,[5] we have to work out two kinds of the transition processes of the above nature; one is the direct process (the second order transition) in which one phonon is emitted together with the simultaneous Umklappung of nuclear spin, and the other the Raman process (the third order one) in which one phonon is emitted and another phonon is absorbed in the nuclear spin Umklappung in a similar way to the scattering process of light.* At first sight, one would expect the direct process to be the most predominant one as it is a process of the second order in contrast with the Raman process. But all lattice waves can cause a certain transition by the Raman process, whereas the direct process in our case requires a lattice wave of a definite phonon according to the conservation law of energy. Further, the number of the Raman process rises rapidly with the temperatures. At higher temperatures, therefore, the Raman process will be expected to be the more predominant one, while, at lower temperatures, the direct process will predominate. In the present paper (Part I) we shall confine ourselves to the direct process of the nuclear spin-lattice relaxation and in Part II the Raman process shall be dealt with.

§ 2. General formulation of nuclear spin-lattice relaxation due to lattice vibrations

We shall consider the system of nuclear spins in combination with the systems of crystal electrons and lattice vibrations. The total Hamiltonian for our problem, therefore, may be written as

---

* In the theory of paramagnetic relaxation due to Van Vleck the similar processes have been worked out although the detailed structures of the transition process are essentially different from ours.

$$\mathfrak{H}=\mathfrak{H}_N+\mathfrak{H}_e+\mathfrak{H}_L+\mathfrak{H}_{NN'}+\partial\mathfrak{H}_{NL}+\partial\mathfrak{H}_{Ne}+\partial\mathfrak{H}_{eL}+\partial\mathfrak{H}'. \tag{1}$$

Here $\mathfrak{H}_N$ denotes the system of nuclear spins in an external magnetic field $\vec{H}$, being expressed by

$$\mathfrak{H}_N=-\mu_N\sum_i\vec{\sigma}_i\vec{H}, \tag{2}$$

in which $\mu_N\vec{\sigma}_i$ is the nuclear magnetic moment operator of a nucleus situated at the i-th lattice point within the crystal and $\vec{\sigma}_i$ the well-known Pauli spin matrix vector. We shall here suppose, for simplicity, the magnitude of a nuclear spin to have $1/2$ since the following computations are aimed to give an order of magnitude for the spin-lattice relaxation time and, further, they are easily generalized to the case of the nuclear spin greater than $1/2$.

For the crystal electron in the periodic field $V(\vec{r})$, it follows, as usual,

$$\mathfrak{H}_e=-\hbar^2/2m\cdot\Delta+V(\vec{r}), \tag{3}$$

where Δ denotes Laplacian operator with respect to electronic coordinates and m the electronic mass, $\hbar$ Planck's constant divided by 2π. Since we adopt, for convenience, Wilson's insulator model for the crystalline solids,[11] the electronic energy band system is supposed to be consisted of a filled band and an unoccupied one in the neighbourhood of the Fermi energy, two bands being separated from each other by a forbidden region of finite breadth. The corresponding eigenfunctions and energies shall be given in the next chapter.

$\mathfrak{H}_L$ is the energy of lattice vibrations, which is expressed by

$$\mathfrak{H}_L=\sum_{\vec{q}i}(N_{\vec{q}i}+1/2)\hbar\omega_{\vec{q}i}, \tag{4}$$

$\vec{q}$ denotes a wave number vector, i specifies each of the polarizations of phonon ($i=1$, longitudinal and $i=2$, 3, transverse ones), $\hbar\omega_{\vec{q}i}$ a phonon quantum and $N_{\vec{q}i}$ the number of a phonon specified by $\vec{q}$ and i. Its average value at thermal equilibrium is governed by Planck's law.

$$N_{\vec{q}i}=(\exp(\hbar\omega_{\vec{q}i}/kT)-1)^{-1}, \tag{5}$$

where k expresses Boltzmann constant and T the absolute temperature.

The sum of the magnetic dipolar interactions between the nuclear spins l and l' will be given by

$$\mathfrak{H}_{NN'}=\sum_{l>l'}\mu_N^2(\vec{\sigma}_l\cdot\vec{\sigma}_{l'}/R_{ll'}^3-3(\vec{\sigma}_l\cdot\vec{R}_{ll'})(\vec{\sigma}_{l'}\cdot\vec{R}_{ll'})/R_{ll'}^5). \tag{6}$$

$R_{ll'}$ designates the mutual distance between the equilibrium positions of the lattice points l and l'.

Since the mutual distance between any two nuclear spins may be influenced by the thermal vibrations of crystal lattice, a part of the nuclear magnetic dipolar interactions dependent upon the thermal displacement of lattice points may be written as

$$\partial\mathfrak{H}_{NL}=\sum_x\sum_{ll'}\partial\mathfrak{H}_{NN',ll'}/\partial X_{ll'}\cdot u_{ll',x}+\text{the second order term}, \tag{7}$$

where $\mathfrak{H}_{NN',ll'}$ denotes a summand in (6), $X_{ll'}$ the x-component of $\vec{R}_{ll'}$, $u_{ll',x}$ the difference of the x-components of two thermal displacement vectors of lattice points l and l'. The coupling (7) is well-known to be responsible for a possible mode of energy transformation between the nuclear spin system and the lattice vibrations, which coupling has actually been taken into account in Waller's theory[10] of spin-lattice relaxation.

Similarly, the magnetic dipolar interaction between the nuclear spin situated at $\vec{R}_l$ and the crystal electron spin takes the following form

$$\delta\mathfrak{H}_{Ne}=\mu_N\mu_e(\vec{\sigma}_N\cdot\vec{\sigma}_e/|\vec{r}-\vec{R}_l|^3-3(\vec{\sigma}_N\cdot(\vec{r}-\vec{R}_l))(\vec{\sigma}_e\cdot(\vec{r}-\vec{R}_l))/|\vec{r}-\vec{R}_l|^5). \qquad (8)$$

Here $\mu_e\vec{\sigma}_e$ and $\mu_N\vec{\sigma}_N$ designate the magnetic moment operators of an electron and a nucleus respectively, and $\vec{r}$ the position vector of a crystal electron.

Finally, the mutual interaction of crystal electron with the lattice vibrations may be expressed by

$$\delta\mathfrak{H}_{eL}=-\vec{u}\,\mathrm{grad}\,V(\vec{r})+1/2(\vec{u}\,\mathrm{grad})(\vec{u}\,\mathrm{grad})V(\vec{r})+\cdots\cdots, \qquad (9)$$

as is well-known in the theory of electrical conductivity in solids.[11] In (9) the deformable ion model has been adopted and $\vec{u}$ is the thermal displacement vector, being expressed by

$$\vec{u}=G^{-3/2}\sum_{\vec{q}i}\vec{e}_{\vec{q}i}(a_{\vec{q}i}\exp(i\vec{q}\vec{r})+a^*_{\vec{q}i}\exp(-i\vec{q}\vec{r})), \qquad (10)$$

in which G^3 denotes the total number of atoms involved in the crystal, $\vec{e}_{\vec{q}i}$ the polarization unit vector of a phonon specified by $\vec{q}$ and i. $a_{\vec{q}i}$ and $a^*_{\vec{q}i}$ are the emission and absorption operators of a phonon, whose nonvanishing matrix elements are

$$(N_{\vec{q}i}|a_{\vec{q}i}|N_{\vec{q}i}-1)=(N_{\vec{q}i}-1|a^*_{\vec{q}i}|N_{\vec{q}i})=\sqrt{\hbar N_{\vec{q}i}/2M\omega_{\vec{q}i}}. \qquad (11)$$

$\delta\mathfrak{H}'$ represents all the remaining interactions, which do not concern us here.

As easily seen, the order of magnitude of the magnetic dipolar interactions among the nuclear spins ($\mathfrak{H}_{NN'}$) becomes $U_0=\mu_N^2/(\text{lattice constant})^3\sim10^{-22}$, while the magnetic energy of a nuclear spin itself is found to be $V_0=\mu_N H\sim10^{-23}H$. Therefore, as far as the following condition,

$$U_0\ll V_0, \qquad \therefore \quad H\gtrsim 10 \text{ gauss},$$

is valid, we are permitted to treat approximately the nuclear spin system as a decoupled one and the effect due to the coupling (6) may be approximately represented by an appropriate, local magnetic field acted upon the nuclear spin.

As shown in Waller's theory for the spin-lattice relaxation, the nuclear magnetic relaxation due to the coupling (7) becomes remarkably slower so that the available experimental results can not be accounted for satisfactorily. Furthermore, since we are now considering the nuclear spin system embedded within the non-metallic crystal, the coupling (8) alone can not be useful for the nuclear spin-lattice relaxation on account of the energy conservation being invalid in such case.

In view of the above situations we shall here propose for the nuclear spin-lattice

relaxation to be induced through the second or the third order transition processes due to the sum of the couplings (8) and (9), i. e.,

$$\delta\mathfrak{H}=\delta\mathfrak{H}_{eL}+\delta\mathfrak{H}_{Ne}\,, \tag{12}$$

in which the crystal electrons may be supposed to take part in the intermediate transitions alone.*

Thus we have

$$(i\,|\,\delta\mathfrak{H}\,|f)=\sum_{j}\frac{(i\,|\,\delta\mathfrak{H}\,|j)\,(j\,|\,\delta\mathfrak{H}\,|f)}{E_i-E_j} \tag{13}$$

for the second order process and

$$(i\,|\,\delta\mathfrak{H}\,|f)=\sum_{jj'}\frac{(i\,|\,\delta\mathfrak{H}\,|j)\,(j\,|\,\delta\mathfrak{H}\,|j')\,(j'\,|\,\delta\mathfrak{H}\,|f)}{(E_i-E_j)\,(E_i-E_{j'})}$$
$$+\sum_{j}\left\{\frac{(i\,|\,\delta\mathfrak{H}''\,|j)\,(j\,|\,\delta\mathfrak{H}\,|f)}{E_i-E_j}+\frac{(i\,|\,\delta\mathfrak{H}\,|j)\,(j\,|\,\delta\mathfrak{H}''\,|f)}{E_i-E_j}\right\}, \tag{14}$$

for the third order one, where i and f designate the initial and final states, and j, j' the intermediate ones. Further, E_i, E_j and $E_{j'}$ are the corresponding energies of the unperturbed system. $\delta\mathfrak{H}''$ represents the second order term of $\delta\mathfrak{H}_{eL}$ in (9).

Now, for the former case, the nuclear spin-Umklappung may be considered to be accompanied by the emission of a single phonon, whereas, for the latter, to be accompanied by the emission of one phonon and the absorption of another phonon simultaneously, on account of which we shall designate the former by the direct process and the latter by the Raman process in the following. The energy conservations corresponding to the above two cases will be represented by

$$2\mu_N H=\hbar\omega_q \tag{15}$$

and

$$2\mu_N H=\hbar(\omega_q-\omega_{q'}) \tag{16}$$

respectively.

According to the general theory of quantum mechanics, the transition probabilities of spin-Umklappung for *any* nuclear spin involved in the crystalline solids may be written as

$$W_d=\frac{2\pi}{\hbar}\,G^3\left(\frac{G\alpha}{2\pi}\right)^6\frac{\omega_q^2}{\hbar}\int_0^{2\pi}d\phi_q\int_0^{\pi}\sin\theta_q d\theta_q\sum_{i}\frac{1}{u_i^3}\,2\int_{-\pi/\alpha}^{\pi/\alpha}d\vec{k}\,|\,(i\,|\,\delta\mathfrak{H}\,|f)\,|^2 \tag{17}$$

for the direct process and

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* To proceed a systematic computation of the problem according to the order of magnitudes of the various interactions, we should take into consideration the magnetic dipolar interactions among the electron spins themselves, which case will require us to treat all the crystal electron spins as a single coupled system. Still in this case, the transition process under consideration will be actually realized through the interactions described in (12) of the text. The whole procedure of computing the transition probabilities is quite similar to those of our case of Hartree approximation for the crystal electrons and the essentially similar results regarding the relaxation times should be expected.

$$W_r = \frac{2\pi}{\hbar} G^3 \left(\frac{Ga}{2\pi}\right)^9 \frac{1}{\hbar} \int_{2\mu_N H/\hbar}^{k\Theta/\hbar} d\omega_q (\omega_q - 2\mu_N H/\hbar)^2 \omega_q^2 \int_0^{2\pi} d\phi_q \int_0^{\pi} \sin\theta_q d\theta_q \int_0^{2\pi} d\phi_{q'} \int_0^{\pi} \sin\theta_{q'} d\theta_{q'}$$

$$\times \sum_{ii'} \frac{1}{u_i^3 u_{i'}^3} \cdot 2 \int_{-\pi/a}^{\pi/a} d\vec{k} |(i|\delta\mathfrak{H}|f)|^2 \qquad (18)$$

for the Raman process respectively, in which $\sin\theta_q d\theta_q d\phi_q$ and $\sin\theta_{q'} d\theta_{q'} d\phi_{q'}$ denote the solid angles along the direction of propagation of an emitted phonon and that of an absorbed phonon during the Umklapp-process of *any* nuclear spin within the solids. The integration over $\vec{k}$ means allowing for all the contributions from the electrons in the filled band to the mentioned transition probabilities. The factor 2 before the $\vec{k}$-integration is the statistical weight due to the electron spin of each level of electronic energy band in the crystal. The state densities of the final states, to which the transition probabilities are proportional, are easily found to become

$$\rho_E = (Ga/2\pi)^3 \omega_q^2/\hbar^2 u_i^3 \cdot \sin\theta_q d\theta_q d\phi_q$$

for the direct process and

$$\rho_E = (Ga/2\pi)^6 \omega_q^2 \omega_{q'}^2/\hbar^2 u_i^3 u_{i'}^3 \cdot \sin\theta_q d\theta_q d\phi_q \sin\theta_{q'} d\theta_{q'} d\phi_{q'} d\hbar\omega_q$$

for the Raman process respectively, which relations have been made use of in the above expressions (17) and (18). For the Raman process the contributions from all phonons are taken into account in accordance with the conservation law, as expressed by the integration over ω_q, the range of integration being restricted by the energy conservation (16). Furthermore, u_i represents the propagation velocity of a phonon specified by i, and a the lattice constant.

As far as $2\mu_N H \ll kT$, the spin-lattice relaxation time T_1 may be represented by

$$1/2\, T_1 = W_d + W_r, \qquad (19)$$

as shown by Bloembergen, Purcell and Pound.[12] Generally speaking, however, the direct process will predominate at very low temperature ($W_d \gg W_r$) but at higher temperatures the Raman process will be the more frequent one ($W_d \ll W_r$).

§ 3. Matrix elements involved in the direct transition process

For the general formulation of the theory of spin-lattice relaxation in crystalline solids we shall here adopt the simplified model of crystalline insulators due to Wilson, in which the highest filled band is supposed to be of ns one and the lowest unfilled band to be of np one respectively.

The corresponding eigenfunctions and energy values[13] are given by

$$\psi_s(\vec{r}) = G^{-3/2} \sum_{\vec{g}} \phi_s(\vec{r} - a\vec{g}) \exp(i\vec{k}\vec{g}a), \qquad (20)$$

$$E_s(\vec{k}) = E_s + \upsilon_1 - 2\beta_1(\cos ak_1 + \cos ak_2 + \cos ak_3), \qquad (21)$$

and

$$\psi_{pj}(\vec{r}) = G^{-3/2} \sum_{\vec{g}} \phi_{pj}(\vec{r}-a\vec{g}) \exp(i\vec{k}\vec{g}a), \quad (j=x, y, z) \tag{22}$$

$$\left.\begin{aligned} E_{px}(\vec{k}) &= E_p + \alpha_2 + 2\gamma_2 \cos ak_1 - 2\beta_2(\cos ak_2 + \cos ak_3) \\ E_{py}(\vec{k}) &= E_p + \alpha_2 + 2\gamma_2 \cos ak_2 - 2\beta_2(\cos ak_3 + \cos ak_1) \\ E_{pz}(\vec{k}) &= E_p + \alpha_2 + 2\gamma_2 \cos ak_3 - 2\beta_2(\cos ak_1 + \cos ak_2) \end{aligned}\right\}, \tag{23}$$

where $\alpha_1 > 0$, $\alpha_2 > 0$ and $\beta_1 > 0$, $\beta_2 > 0$, $\gamma_2 > 0$ are the energy displacements and the energy breadths due to the interactions of a crystal electron with other ions within the crystal. As is well-known, the above results have been obtained through the Bloch's tightly bound electron approximation method, similar to the Mulliken's *LCAO* method of approximation in molecular structure. ϕ_{pj} and ϕ_s are atomic orbitals around each ion within the crystal, satisfying the following wave equation of a single electron

$$[-\hbar^2/2m \cdot \Delta + U(r)]\phi_s = E_s\phi_s, \quad [-\hbar^2/2m \cdot \Delta + U(r)]\phi_{pj} = E_p\phi_{pj}, \tag{24}$$

in which $U(r)$ denotes the potential energy due to an ion within the crystal, and E_s and E_p are atomic energies belonging to ns and np levels respectively. As usual in the central field of force $U(r)$, the atomic orbitals may be written as

$$\left.\begin{aligned} \phi_s(r) &= R_s(r)/\sqrt{4\pi}, \quad \phi_{px}(\vec{r}) = R_p(r) \cdot x/r \cdot \sqrt{3/4\pi} \\ &\phi_{py}(\vec{r}) = R_p(r) \cdot y/r \cdot \sqrt{3/4\pi} \\ &\phi_{pz}(\vec{r}) = R_p(r) \cdot z/r \cdot \sqrt{3/4\pi} \end{aligned}\right\}, \tag{25}$$

in which $R_s(r)$ and $R_p(r)$ denote the normalized radial eigenfunctions corresponding to ns- and np-levels respectively.

Furthermore, the crystal field $V(r)$ may be considered to be given by

$$V(r) = \sum_{\vec{g}} U(\vec{r}-a\vec{g}),$$

in which $\vec{g}$ specifies each of the lattice sites occupied by ions within the crystal.

The matrix elements of $\partial\mathfrak{H}_{Ne}$ and $\partial\mathfrak{H}_{eL}$ requisite for the direct process are easily seen to be of the following type

$$(m_n, m_s, E_s(\vec{k}) | \partial\mathfrak{H}_{Ne} | m_n', m_s, E_{pj}(\vec{k}')),$$

$$(m_n, m_s, E_{pj}(\vec{k}') | \partial\mathfrak{H}_{Ne} | m_n', m_s, E_s(\vec{k})),$$

$$(E_{pj}(\vec{k}'), N_{\vec{q}} | \partial\mathfrak{H}_{eL} | E_s(\vec{k}), N_{\vec{q}} \pm 1)$$

and

$$(E_s(\vec{k}), N_{\vec{q}} | \partial\mathfrak{H}_{eL} | E_{pj}(\vec{k}'), N_{\vec{q}} \pm 1),$$

in which m_n, m_n' denote the magnetic quantum numbers of a nuclear spin before and after the transition, and m_s the magnetic quantum number of a crystal electron respectively.

By the use of (8), (20) and (22), we obtain

$$(m_n,\ m_s,\ E_s(\vec{k})\,|\,\delta\mathfrak{H}_{Ne}\,|\,m_n',\ m_s,\ E_{pj}(\vec{k}'))$$
$$=G^{-3}\mu_e\mu_N\sum_{\vec{g}\,\vec{g}'}\exp(-i(\vec{k}'\vec{g}'-\vec{k}\vec{g})a)$$
$$\times\{(m_n|\vec{\sigma}_N|m_n')(m_s|\vec{\sigma}_e|m_s)A_j(\vec{g},\vec{g}')-3B_j(\vec{g},\vec{g}')\},\tag{26}$$

where

$$A_j(\vec{g},\vec{g}')=\int\phi_s(\vec{r}-a\vec{g})\phi_{pj}(\vec{r}-a\vec{g}')/|\vec{r}-a\vec{n}|^3\cdot d\tau\,,\tag{27}$$

$$B_j(\vec{g},\vec{g}')=\int\Big(\frac{\vec{r}-a\vec{n}}{|\vec{r}-a\vec{n}|}\cdot(m_s|\vec{\sigma}_e|m_s)\Big)\Big(\frac{\vec{r}-a\vec{n}}{|\vec{r}-a\vec{n}|}\cdot(m_n|\vec{\sigma}_N|m_n')\Big)$$
$$\times\frac{\phi_s(\vec{r}-a\vec{g})\phi_{pj}(\vec{r}-a\vec{g}')}{|\vec{r}-a\vec{n}|^3}d\tau\,,\tag{28}$$

and $\vec{n}$ denotes the specified lattice point on which the nuclear spin under consideration is situated.

Since, as easily seen, we have $A_j(\vec{n},\vec{n})=B_j(\vec{n},\vec{n})=0$, the most predominant $A_j(\vec{g},\vec{g}')$ and $B_j(\vec{g},\vec{g}')$ shall be taken into consideration, in the following, among the various quantities of $A_j(\vec{g},\vec{g}')$ and $B_j(\vec{g},\vec{g}')$ belonging to the nearest neighbour-pairs of $\vec{g}$ and $\vec{g}'$ with respect to $\vec{n}$, the less significant ones being neglected approximately.

Thus, it follows

$$A_x(\vec{n},\vec{n}\pm\vec{i})=A_y(\vec{n},\vec{n}\pm\vec{j})=A_z(\vec{n},\vec{n}\pm\vec{k})$$
$$=\pm\frac{\sqrt{3}}{2}\int_0^\infty d\rho\int_{-\infty}^{\infty}dz\,R_s(\sqrt{\rho^2+z^2})R_p(\sqrt{\rho^2+(z-a)^2})\frac{\rho(z-a)}{(\rho^2+z^2)^{3/2}(\rho^2+(z-a)^2)^{1/2}}\tag{29}$$

and

$$A_x(\vec{n}\pm\vec{i},\vec{n})=A_y(\vec{n}\pm\vec{j},\vec{n})=A_z(\vec{n}\pm\vec{k},\vec{n})$$
$$=\pm\frac{\sqrt{3}}{2}\int_0^\infty d\rho\int_{-\infty}^{\infty}dz\,R_s(\sqrt{\rho^2+(z-a)^2})R_p(\sqrt{\rho^2+z^2})\frac{\rho z}{(\rho^2+z^2)^2}\,,\tag{30}$$

in which the cylindrical coordinates (z,ρ,φ) are adopted and the integration with respect to φ has been carried through in the above expressions. Further, $\vec{i}$, $\vec{j}$, $\vec{k}$ denote the unit vectors along the principal axes of the crystal.

Similarly, we have

$$B_x(\vec{n},\vec{n}\pm\vec{i})=\pm\frac{3}{4}\Big\{(m_s|\sigma_{ey}|m_s)(m_n|\sigma_{Ny}|m_n')+(m_s|\sigma_{ez}|m_s)(m_n|\sigma_{Nz}|m_n')\Big\}\cdot J_1$$
$$\pm\frac{3}{2}(m_s|\sigma_{ex}|m_s)(m_n|\sigma_{Nx}|m_n')J_2\,,\tag{31}$$

$$B_y(\vec{n},\vec{n}\pm\vec{j})=\pm\frac{3}{4}\Big\{(m_s|\sigma_{ez}|m_s)(m_n|\sigma_{Nz}|m_n')+(m_s|\sigma_{ex}|m_s)(m_n|\sigma_{Nx}|m_n')\Big\}\cdot J_1$$

$$\pm\frac{3}{2}(m_s|\sigma_{ey}|m_s)(m_n|\sigma_{Ny}|m_n')J_2, \tag{32}$$

$$B_z(\vec{n},\vec{n}\pm\vec{k})=\pm\frac{3}{4}\left\{(m_s|\sigma_{ex}|m_s)(m_n|\sigma_{Nx}|m_n')+(m_s|\sigma_{ey}|m_s)(m_n|\sigma_{Ny}|m_n')\right\}\cdot J_1$$

$$\pm\frac{3}{2}(m_s|\sigma_{ez}|m_s)(m_n|\sigma_{Nz}|m_n')J_2, \tag{33}$$

$$J_1=\frac{1}{\sqrt{3}}\int_0^\infty d\rho\int_{-\infty}^\infty dz\,R_s(\sqrt{\rho^2+z^2})R_p(\sqrt{\rho^2+(z-a)^2})\frac{\rho^3(z-a)}{(\rho^2+z^2)^{5/2}(\rho^2+(z-a)^2)^{1/2}}, \tag{34·1}$$

$$J_2=\frac{1}{\sqrt{3}}\int_0^\infty d\rho\int_{-\infty}^\infty dz\,R_s(\sqrt{\rho^2+z^2})R_p(\sqrt{\rho^2+(z-a)^2})\frac{\rho z^2(z-a)}{(\rho^2+z^2)^{5/2}(\rho^2+(z-a)^2)^{1/2}}, \tag{34·2}$$

and

$$B_x(\vec{n}\pm\vec{i},\vec{n})=\pm\frac{3}{4}\left\{(m_s|\sigma_{ey}|m_s)(m_n|\sigma_{Ny}|m_n')+(m_s|\sigma_{ez}|m_s)(m_n|\sigma_{Nz}|m_n')\right\}K_1$$

$$\pm\frac{3}{2}(m_s|\sigma_{ex}|m_s)(m_n|\sigma_{Nx}|m_n')K_2, \tag{35}$$

$$B_y(\vec{n}\pm\vec{j},\vec{n})=\pm\frac{3}{4}\left\{(m_s|\sigma_{ez}|m_s)(m_n|\sigma_{Nz}|m_n')+(m_s|\sigma_{ex}|m_s)(m_n|\sigma_{Nx}|m_n')\right\}K_1$$

$$\pm\frac{3}{2}(m_s|\sigma_{ey}|m_s)(m_n|\sigma_{Ny}|m_n')K_2, \tag{36}$$

$$B_z(\vec{n}\pm\vec{k},\vec{n})=\pm\frac{3}{4}\left\{(m_s|\sigma_{ex}|m_s)(m_n|\sigma_{Nx}|m_n')+(m_s|\sigma_{ey}|m_s)(m_n|\sigma_{Ny}|m_n')\right\}K_1$$

$$\pm\frac{3}{2}(m_s|\sigma_{ez}|m_s)(m_n|\sigma_{Nz}|m_n')K_2, \tag{37}$$

$$K_1=\frac{1}{\sqrt{3}}\int_0^\infty d\rho\int_{-\infty}^\infty dz\,R_s(\sqrt{\rho^2+(z-a)^2})R_p(\sqrt{\rho^2+z^2})\frac{\rho^3 z}{(\rho^2+z^2)^3}, \tag{38·1}$$

$$K_2=\frac{1}{\sqrt{3}}\int_0^\infty d\rho\int_{-\infty}^\infty dz\,R_s(\sqrt{\rho^2+(z-a)^2})R_p(\sqrt{\rho^2+z^2})\frac{\rho z^3}{(\rho^2+z^2)^3}. \tag{38·2}$$

Since each axis of the coordinate system (x, y, z) is along each of the principal axes of the crystal and that of (X, Y, Z) is supposed to be the quantization coordinate system of nuclear spin, Z being along the direction of an external magnetic field $\vec{H}$, the direction cosines of the former with respect to the latter shall be represented by (l_1, l_2, l_3), (m_1, m_2, m_3) and (n_1, n_2, n_3) respectively.

Thus, we have

$$\left.\begin{aligned}\sigma_x&=l_1\sigma_X+l_2\sigma_Y+l_3\sigma_Z\\ \sigma_y&=m_1\sigma_X+m_2\sigma_Y+m_3\sigma_Z\\ \sigma_z&=n_1\sigma_X+n_2\sigma_Y+n_3\sigma_Z\end{aligned}\right\}, \tag{39·1}$$

and

$$\sigma_X=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \sigma_Y=\begin{pmatrix}0&-i\\i&0\end{pmatrix},\quad \sigma_Z=\begin{pmatrix}1&0\\0&-1\end{pmatrix}. \tag{39·2}$$

Taking into account (39·1) and (39·2), we have, after a simple evaluation,

$$\left.\begin{aligned}&(\pm1/2|\sigma_{ey}|\pm1/2)(-1/2|\sigma_{Ny}|1/2)+(\pm1/2|\sigma_{ex}|\pm1/2)(-1/2|\sigma_{Nx}|1/2)\\&\qquad=\mp l_3(l_1-il_2)\\&(\pm1/2|\sigma_{ex}|\pm1/2)(-1/2|\sigma_{Nx}|1/2)=\pm l_3(l_1-il_2)\end{aligned}\right\}, \tag{40·1}$$

$$\left.\begin{aligned}&(\pm1/2|\sigma_{ex}|\pm1/2)(-1/2|\sigma_{Nz}|1/2)+(\pm1/2|\sigma_{ex}|\pm1/2)(-1/2|\sigma_{Nx}|1/2)\\&\qquad=\mp m_3(m_1-im_2)\\&(\pm1/2|\sigma_{ey}|\pm1/2)(-1/2|\sigma_{Ny}|1/2)=\pm m_3(m_1-im_2)\end{aligned}\right\}, \tag{40·2}$$

$$\left.\begin{aligned}&(\pm1/2|\sigma_{ex}|\pm1/2)(-1/2|\sigma_{Nx}|1/2)+(\pm1/2|\sigma_{ey}|\pm1/2)(-1/2|\sigma_{Ny}|1/2)\\&\qquad=\mp n_3(n_1-in_2)\\&(\pm1/2|\sigma_{ez}|\pm1/2)(-1/2|\sigma_{Nz}|1/2)=\pm n_3(n_1-in_2)\end{aligned}\right\}, \tag{40·3}$$

and, further,

$$(m_n|\vec{\sigma}_N|m_n')(m_s|\vec{\sigma}_s|m_s)=0\,.\quad (m_n\neq m_n') \tag{41}$$

Substituting the equations of (29)–(37), (40·1)–(40·3) and (41) into the expression (26), we get finally, for the required matrix elements,

$$\begin{aligned}&(-1/2,\ m_s,\ E_s(\vec{k})|\delta\mathfrak{H}_{Ne}|1/2,\ m_s,\ E_{px}(\vec{k}'))=9/2\cdot iG^{-3}\mu_e\mu_N\exp(-i(\vec{k}'-\vec{k})\vec{n}a)\\&\quad\times\{\pm l_3(l_1-il_2)\}\{[J\cos(k_x'-k_x)a-K]\sin k_xa+J\sin(k_x'-k_x)a\cdot\cos k_xa\},\end{aligned} \tag{42·1}$$

$$\begin{aligned}&(-1/2,\ m_s,\ E_s(\vec{k})|\delta\mathfrak{H}_{Ne}|1/2,\ m_s,\ E_{py}(\vec{k}'))=9/2\cdot iG^{-3}\mu_e\mu_N\exp(-i(\vec{k}'-\vec{k})\vec{n}a)\\&\quad\times\{\pm m_3(m_1-im_2)\}\{[J\cos(k_y'-k_y)a-K]\sin k_ya+J\sin(k_y'-k_y)a\cdot\cos k_ya\},\end{aligned} \tag{42·2}$$

$$\begin{aligned}&(-1/2,\ m_s,\ E_s(\vec{k})|\delta\mathfrak{H}_{Ne}|1/2,\ m_s,\ E_{pz}(\vec{k}'))=9/2\cdot iG^{-3}\mu_e\mu_N\exp(-i(\vec{k}'-\vec{k})\vec{n}a)\\&\quad\times\{\pm n_3(n_1-in_2)\}\{[J\cos(k_z'-k_z)a-K]\sin k_za+J\sin(k_z'-k_z)a\cdot\cos k_za\},\end{aligned} \tag{42·3}$$

$$\begin{aligned}&(-1/2,\ m_s,\ E_{px}(\vec{k}')|\delta\mathfrak{H}_{Ne}|1/2,\ m_s,\ E_s(\vec{k}))=-9/2\cdot iG^{-3}\mu_e\mu_N\exp((i\vec{k}'-\vec{k})\vec{n}a)\\&\quad\times\{\pm l_3(l_1-il_2)\}\{[J(k_x'-k_x)a-K]\sin k_xa+J\sin(k_x'-k_x)a\cdot\cos k_xa\},\end{aligned} \tag{42·4}$$

$$(-1/2,\ m_s,\ E_{py}(\vec{k}')|\delta\mathfrak{H}_{Ne}|1/2,\ m_s,\ E_s(\vec{k}))=-9/2\cdot iG^{-3}\mu_e\mu_N\exp(i(\vec{k}'-\vec{k})\vec{n}a)$$
$$\times\{\pm m_3(m_1-im_2)\}\{[J\cos(k_y'-k_y)a-K]\sin k_y a+J\sin(k_y'-k_y)a\cdot\cos k_y a\}, \tag{42·5}$$

$$(-1/2,\ m_s,\ E_{pz}(\vec{k}')|\delta\mathfrak{H}_{Ne}|1/2,\ m_s,\ E_s(\vec{k}))=-9/2\cdot iG^{-3}\mu_e\mu_N\exp(i(\vec{k}'-\vec{k})\vec{n}a)$$
$$\times\{\pm n_3(n_1-in_2)\}\{[J\cos(k_z'-k_z)a-K]\sin k_z a+J\sin(k_z'-k_z)a\cdot\cos k_z a\}, \tag{42·6}$$

where

$$J=2J_2-J_1=\frac{1}{\sqrt{3}}\int_0^\infty d\rho\int_{-\infty}^{\infty}dz\,R_s(\sqrt{\rho^2+z^2})R_p(\sqrt{\rho^2+(z-a)^2})$$
$$\times\frac{\rho(z-a)(2z^2-\rho^2)}{(\rho^2+(z-a)^2)^{1/2}(\rho^2+z^2)^{5/2}}, \tag{43·1}$$

$$K=2K_2-K_1=-\frac{1}{\sqrt{3}}\int_0^\infty d\rho\int_{-\infty}^{\infty}dz\,R_s(\sqrt{\rho^2+(z-a)^2})R_p(\sqrt{\rho^2+z^2})\frac{\rho z(2z^2-\rho^2)}{(\rho^2+z^2)^3}. \tag{43·2}$$

The actual evaluations of J and K may be carried out through the rather lengthy but elementary procedure, which results shall be described in the Appendix.

The matrix elements of the first term in (9) may be written as

$$(E_{pj}(\vec{k}'),\ N_{\vec{q}}|\delta\mathfrak{H}_{eL}|E_s(\vec{k}),\ N_{\vec{q}}\pm 1)=-G^{-3/2}\sqrt{\hbar(\overrightarrow{N_q}+\tfrac{0}{1})/2M\omega_{qi}}\cdot K_j, \tag{44}$$

with

$$K_j=\int\psi_{pj}(\vec{r})(\vec{e}_{\vec{q}i}\,\mathrm{grad}\,V(\vec{r}))\psi_s^*(\vec{r})\exp(\mp i\vec{q}\vec{r})d\tau, \tag{44·1}$$

by using of (10) and (11). Putting (20), (22) into (44·1), it follows*

$$K_j=G^{-3}\sum_{\vec{n}}\sum_{\vec{m}}\sum_{\vec{m}'}\int\phi_s(\vec{r}+\vec{m}a)(\vec{e}_{\vec{q}i}\,\mathrm{grad}\,U(r))\phi_{pj}(\vec{r}+\vec{m}'a)\exp(\mp i\vec{q}\vec{r}+i(\vec{k}'-\vec{k})a\vec{n}$$
$$+i(\vec{k}\vec{m}-\vec{k}'\vec{m}')a)d\tau.$$

The most predominant contribution to K_j is easily seen to come from the term with a maximum overlapping of atomic orbitals $\phi_s(\vec{r}+\vec{m}a)$ and $\phi_{pj}(\vec{r}+\vec{m}'a)$, namely, the one denoted by $\vec{m}=\vec{m}'=0$. Neglecting approximately the less significant summands in the above expression, we get approximately

$$K_j=G^{-3}\sum_{\vec{n}}\exp(i(\vec{k}'-\vec{k}\mp\vec{q})\vec{n}a)\int\phi_s(\vec{r})(\vec{e}_{\vec{q}i}\,\mathrm{grad}\,U(r))\phi_{pj}(\vec{r})\exp(\mp i\vec{q}\vec{r})d\tau_0$$
$$=\int\phi_s(\vec{r})(\vec{e}_{\vec{q}i}\,\mathrm{grad}\,U(r))\phi_{pj}(\vec{r})\exp(\mp i\vec{q}\vec{r})d\tau_0\cdot\delta_{\vec{k}',\vec{k}\pm\vec{q}}.$$

As seen from the conservation law of energy, $2\mu_N H=\hbar\omega_{qi}=\hbar u_i q$, the wave length $1/q$ of the emitted phonon becomes much larger than the atomic dimension on account

* The coordinate origin is situated on the $\vec{n}$-th lattice site.

of the smallness of $2\mu_N H$ in our case, which situation leads to $\exp(\mp i\vec{q}\vec{r})$ 1 in the above integral of K_j. Furthermore, on making use of the well-known relation

$$\int \phi_s(\vec{r})\vec{e}_{\vec{q}i}\,\mathrm{grad}\,U(r)\phi_{pj}(\vec{r})\,d\tau = m/\hbar^2\cdot(E_p-E_s)^2\int\phi_s(\vec{r})(\vec{e}_{\vec{q}i}\vec{r})\phi_{pj}(\vec{r})\,d\tau\,,$$

we obtain finally

$$(E_{pj}(\vec{k}'),\ N_{\vec{q}}|\delta\mathfrak{H}_{eL}|E_s(\vec{k}),\ N_{\vec{q}}\pm 1) = -G^{-3/2}\sqrt{\hbar(N_q+\tfrac{1}{0})/2M\omega_{qt}}\cdot m/\hbar^2\cdot(E_p-E_s)^2$$
$$\times\int\phi_{pj}(\vec{r})(\vec{e}_{\vec{q}i}\vec{r})\phi_s(\vec{r})\,d\tau\cdot\delta_{\vec{k}',\,\vec{k}\pm\vec{q}}\,. \qquad (45\cdot 1)$$

Similarly we have

$$(E_s(k),\ N_{\vec{q}}|\delta\mathfrak{H}_{eL}|E_{pj}(\vec{k}'),\ N_{\vec{q}}\pm 1) = -G^{-3/2}\sqrt{\hbar(N_q+\tfrac{1}{0})/2M\omega_{qt}}\cdot m/\hbar^2\cdot(E_p-E_s)^2$$
$$\times\int\phi_{pj}(\vec{r})(\vec{e}_{\vec{q}i}\vec{r})\phi_s(\vec{r})\,d\tau\cdot\delta_{\vec{k},\,\vec{k}'\pm\vec{q}}\,. \qquad (45\cdot 2)$$

§ 4. Transition probabilities of the direct process

The transition matrix element in the direct process under consideration may be written, from (13), as

$$(i|\delta\mathfrak{H}|f)$$
$$=\sum_{j=x,y,z}\frac{(-1/2,\,m_s,\,E_s(\vec{k})|\delta\mathfrak{H}_{Ne}|1/2,\,m_s,\,E_{pj}(\vec{k}+\vec{q}))(E_{pj}(\vec{k}+\vec{q}),\,N_q|\delta\mathfrak{H}_{eL}|E_s(\vec{k}),\,N_q+1)}{2\mu_N H+E_s(\vec{k})-E_{pj}(\vec{k}+\vec{q})}$$
$$+\sum_{j=x,y,z}\frac{(E_s(\vec{k}),\,N_q|\delta\mathfrak{H}_{eL}|E_{pj}(\vec{k}-\vec{q}),\,N_q+1)(-1/2,\,m_s,\,E_{pj}(\vec{k}-\vec{q})|\delta\mathfrak{H}_{Ne}|1/2,\,m_s,\,E_s(\vec{k}))}{-\hbar\omega_{qt}+E_s(\vec{k})-E_{pj}(\vec{k}-\vec{q})}\,,$$

which may be transformed, after substituting (42), (43), and (45) into the above equation, into

$$(i|\delta\mathfrak{H}|f) = \pm L\cdot S\Big\{Xl_3(l_1-il_2)\Big[-\frac{(J\cos q_1a-K)\sin k_1a+J\sin q_1a\cdot\cos k_1a}{2\mu_N H+E_s(\vec{k})-E_{px}(\vec{k}+\vec{q})}$$
$$+\frac{(J\cos q_1a-K)\sin k_1a-J\sin q_1a\cdot\cos k_1a}{-2\mu_N H+E_s(\vec{k})-E_{px}(\vec{k}-\vec{q})}\Big]$$
$$+Ym_3(m_1-im_2)\Big[-\frac{(J\cos q_2a-K)\sin k_2a+J\sin q_2a\cdot\cos k_2a}{2\mu_N H+E_s(\vec{k})-E_{py}(\vec{k}+\vec{q})}$$
$$+\frac{(J\cos q_2a-K)\sin k_2a-J\sin q_2a\cdot\cos k_2a}{-2\mu_N H+E_s(\vec{k})-E_{py}(\vec{k}-\vec{q})}\Big]$$
$$+Zn_3(n_1-in_2)\Big[-\frac{(J\cos q_3a-K)\sin k_3a+J\sin q_3a\cdot\cos k_3a}{2\mu_N H+E_s(\vec{k})-E_{pz}(\vec{k}+\vec{q})}$$
$$+\frac{(J\cos q_3a-K)\sin k_3a-J\sin q_3a\cdot\cos k_3a}{-2\mu_N H+E_s(\vec{k})-E_{pz}(\vec{k}-\vec{q})}\Big]\Big\}, \qquad (46)$$

in which the energy conservation $\hbar\omega_{qi}=2\mu_N H$ has been made use of and the following abbreviations are adopted.

$$L=-G^{-3/2}m/\hbar^2\cdot(E_p-E_s)^2\sqrt{\hbar(N_q+1)/2M\omega_{qi}}\,, \tag{47}$$

$$S=-9/2\cdot iG^{-3}\mu_N\mu_e\exp(i\vec{q}\vec{n}a) \tag{48}$$

and

$$\left.\begin{matrix}X\\Y\\Z\end{matrix}\right\}=\int\phi_s(\vec{r})\,(\vec{e}_{\vec{q}i}\cdot\vec{r})\left\{\begin{matrix}\phi_{px}(\vec{r})\\\phi_{py}(\vec{r})\\\phi_{pz}(\vec{r})\end{matrix}\right\}d\tau\,. \tag{49}$$

Putting (25) into (49), we obtain, after carrying through the angular integrations,

$$X=e_{\vec{q}i,x}R\,,\quad Y=e_{\vec{q}i,y}R\,,\quad Z=e_{\vec{q}i,z}R\,; \tag{50·1}$$

$$R=1/\sqrt{3}\cdot\int_0^\infty R_p(r)R_s(r)r^3dr\,. \tag{50·2}$$

As for the electronic energy band of the crystalline insulator the following relation may be considered to be satisfied;

$$\Delta E=E_p-E_s+u_2-u_1\gg\beta_1,\ \beta_2\ \text{and}\ \gamma_2\,, \tag{51}$$

on account of which the denominators in each term involved in (46) may be expanded into the power series as follows.

$$\left.\begin{aligned}(\pm2\mu_NH+E_s(\vec{k})-E_{px}(\vec{k}\pm\vec{q}))^{-1}&\approx-\{1+(\varepsilon_{\pm1}(\vec{k})\pm2\mu_NH)/\Delta E\\&\quad+(\varepsilon_{\pm1}(\vec{k})\pm2\mu_NH)^2/\Delta E^2\}/\Delta E\\(\pm2\mu_NH+E_s(\vec{k})-E_{py}(\vec{k}\pm\vec{q}))^{-1}&\approx-\{1+(\varepsilon_{\pm2}(\vec{k})\pm2\mu_NH)/\Delta E\\&\quad+(\varepsilon_{\pm2}(\vec{k})\pm2\mu_NH)^2/\Delta E^2\}/\Delta E\\(\pm2\mu_NH+E_s(\vec{k})-E_{pz}(\vec{k}\pm\vec{q}))^{-1}&\approx-\{1+(\varepsilon_{\pm3}(\vec{k})\pm2\mu_NH)/\Delta E\\&\quad+(\varepsilon_{\pm3}(\vec{k})\pm2\mu_NH)^2/\Delta E^2\}/\Delta E\end{aligned}\right\}, \tag{52}$$

with the following abbreviations;

$$\left.\begin{aligned}\varepsilon_{\pm1}(\vec{k})&=-2(\beta_1\cos ak_1+\gamma_2\cos a(k_1\pm q_1))-2(\beta_1\cos ak_2-\beta_2\cos a(k_2\pm q_2))\\&\quad-2(\beta_1\cos ak_3-\beta_2\cos a(k_3\pm q_3))\\\varepsilon_{\pm2}(\vec{k})&=-2(\beta_1\cos ak_1-\beta_2\cos a(k_1\pm q_1))-2(\beta_1\cos ak_2+\gamma_2\cos a(k_2\pm q_2))\\&\quad-2(\beta_1\cos ak_3-\beta_2\cos a(k_3\pm q_3))\\\varepsilon_{\pm3}(\vec{k})&=-2(\beta_1\cos ak_1-\beta_2\cos a(k_1\pm q_1))-2(\beta_1\cos ak_2-\beta_2\cos a(k_2\pm q_2))\\&\quad-2(\beta_1\cos ak_3+\gamma_2\cos a(k_3\pm q_3))\end{aligned}\right\}. \tag{53}$$

On putting (52) and (53) into (46), we obtain

$$\begin{aligned}(i|\delta\mathfrak{H}|f)=\pm L\cdot S/\Delta E^2\cdot\{&XI_3(I_1-iI_2)[\xi_1\sin ak_1(\varepsilon_{+1}(\vec{k})-\varepsilon_{-1}(\vec{k}))+\eta_1\cos ak_1(\varepsilon_{+1}(\vec{k})\\&+\varepsilon_{-1}(\vec{k}))+2\eta_1\Delta E\cos ak_1+4\mu_NH\xi_1\sin ak_1+\xi_1\sin ak_1(\varepsilon_{+1}^2(\vec{k})-\varepsilon_{-1}^2(\vec{k}))\end{aligned}$$

$$+4\mu_N H(\varepsilon_{+1}(\vec{k})+\varepsilon_{-1}(\vec{k}))\big)/\Delta E+\eta_1\cos ak_1\cdot(\varepsilon_{+1}^2(\vec{k})+\varepsilon_{-1}^2(\vec{k})+4\mu_N H(\varepsilon_{+1}(\vec{k})$$
$$-\varepsilon_{-1}(\vec{k}))+8\mu_N^2H^2)/\Delta E]+Ym_3(m_1-im_2)[\xi_2\sin ak_2(\varepsilon_{+2}(\vec{k})-\varepsilon_{-2}(\vec{k}))$$
$$+\eta_2\cos ak_2(\varepsilon_{+2}(\vec{k})+\varepsilon_{-2}(\vec{k}))+2\eta_2\Delta E\cos ak_2+4\mu_N H\xi_2\sin ak_2+\xi_2\sin ak_2(\varepsilon_{+2}^2(\vec{k})$$
$$-\varepsilon_{-2}^2(\vec{k})+4\mu_N H(\varepsilon_{+2}(\vec{k})+\varepsilon_{-2}(\vec{k})))/\Delta E+\eta_2\cos ak_2\cdot(\varepsilon_{+2}^2(\vec{k})+\varepsilon_{-2}^2(\vec{k})$$
$$+4\mu_N H(\varepsilon_{+2}(\vec{k})-\varepsilon_{-2}(\vec{k}))+8\mu_N^2H^2)/\Delta E]+Zn_3(n_1-in_2)[\xi_3\sin ak_3(\varepsilon_{+3}(\vec{k})$$
$$-\varepsilon_{-3}(\vec{k}))+\eta_3\cos ak_3(\varepsilon_{+3}(\vec{k})+\varepsilon_{-3}(\vec{k}))+2\eta_3\Delta E\cos ak_3+4\mu_N H\xi_3\sin ak_3$$
$$+\xi_3\sin ak_3(\varepsilon_{+3}^2(\vec{k})-\varepsilon_{-3}^2(\vec{k})+4\mu_N H(\varepsilon_{+3}(\vec{k})-\varepsilon_{-3}(\vec{k})))/\Delta E+\eta_3\cos ak_3$$
$$\times(\varepsilon_{+3}^2(\vec{k})+\varepsilon_{-3}^2(\vec{k})+4\mu_N H(\varepsilon_{+3}(\vec{k})-\varepsilon_{-3}(\vec{k}))+8\mu_N^2H^2)/\Delta E]\}\,, \tag{54}$$

in which

$$\left.\begin{aligned}\xi_1&=J\cos aq_1-K\,,\quad \eta_1=J\sin aq_1\\ \xi_2&=J\cos aq_2-K\,,\quad \eta_2=J\sin aq_2\\ \xi_3&=J\cos aq_3-K\,,\quad \eta_3=J\sin aq_3\end{aligned}\right\}. \tag{55}$$

On making use of the phonon wave length being much larger than the lattice constant a, i. e., $aq_1\ll 1$, $aq_2\ll 1$, $aq_3\ll 1$, the cosine or sine terms of aq_1, aq_2, aq_3 may be expanded into the power series,

$$\sin aq_1\approx aq_1\,,\quad \cos aq_1\approx 1-(aq_1)^2/2\,,\quad \text{etc.},$$

the higher order small quantities being neglected approximately.

Thus, we have

$$\int_{-\pi/a}^{\pi/a}dk_1\int_{-\pi/a}^{\pi/a}dk_2\int_{-\pi/a}^{\pi/a}dk_2\,|(i\,|\delta\mathfrak{H}|f)\,|^2=|L\cdot S|^2/\Delta E^4\cdot(\pi/a)^3\cdot 16R^2\cdot\{l_3^2(1-l_3^2)e_{\vec{qi},x}^2$$
$$\times[\textstyle\sum_0+(aq_1)^2\sum_1+a^2(q_2^2+q_3^2)\sum_2]+m_3^2(1-m_3^2)e_{\vec{qi},y}^2[\sum_0+(aq_2)^2\sum_1$$
$$+a^2(q_3^2+q_1^2)\textstyle\sum_2]+n_3^2(1-n_3^2)e_{\vec{qi},z}^2[\sum_0+(aq_3)^2\sum_1+a^2(q_1^2+q_2^2)\sum_2]$$
$$+4(l_3^2m_3^2\,e_{\vec{qi},x}\,e_{\vec{qi},y}\,a^2q_1q_2+m_3^2n_3^2\,e_{\vec{qi},y}\,e_{\vec{qi},z}\,a^2q_2q_3+n_3^2l_3^2\,e_{\vec{qi},z}\,e_{\vec{qi},x}\,a^2q_3q_1)\textstyle\sum_3\}\,, \tag{56}$$

where

$$\left.\begin{aligned}\textstyle\sum_0&=4\mu_N^2H^2(J-K)^2,\\ \textstyle\sum_1&=3\gamma_2^2(J-K)^2+[9(\beta_1+\gamma_2)^2+12(\beta_1-\beta_2)^2+\Delta E^2+8\mu_N^2H^2]J^2\\ &\quad-[4\mu_N^2H^2+6\gamma_2(\beta_1+\gamma_2)]J(J-K),\\ \textstyle\sum_2&=2\beta_2^2(J-K)^2,\\ \textstyle\sum_3&=(\beta_2^2+\gamma_2^2)(J-K)^2-2\gamma_2(3\beta_1-2\beta_2+\gamma_2)J(J-K)+[(\beta_1+\gamma_2)^2+(\beta_1-\beta_2)^2\\ &\quad+4(\beta_1+\gamma_2)(\beta_1-\beta_2)]J^2.\end{aligned}\right\} \tag{56·1}$$

The integration of (56) over the directions of propagation of an emitted phonon may be easily carried through by taking account of

$$q_1 = q \sin\theta_q \cos\phi_q = \omega_q / u_i \cdot \sin\theta_q \cos\phi_q = 2\mu_N H/\hbar u_i \cdot \sin\theta_q \cos\phi_q ,$$
$$q_2 = q \sin\theta_q \sin\phi_q = \omega_q / u_i \cdot \sin\theta_q \sin\phi_q = 2\mu_N H/\hbar u_i \cdot \sin\theta_q \sin\phi_q$$

and

$$q_3 = q \cos\theta_q = \omega_q / u_i \cdot \cos\theta_q = 2\mu_N H/\hbar u_i \cdot \cos\theta_q ,$$

together with the directional dependencies of $e_{\vec{q}i,x}$, $e_{\vec{q}i,y}$ and $e_{\vec{q}i,z}$.

After carrying out the above mentioned procedures involved in (17), we obtain finally, for the transition probability of spin-Umklappung for *any* nuclear spin contained within the crystalline solids,

$$W_d = \frac{27}{10} \frac{a^3}{\pi\hbar^6} (\mu_N \mu_e)^2 (2\mu_N H) \frac{m^2}{M} \left(\frac{E_p - E_s}{E_p - E_s + a_2 - a_1} \right)^4 R^2 \frac{\exp(2\mu_N H/kT)}{\exp(2\mu_N H/kT) - 1}$$
$$\times \left\{ \left[l_3^2 (1 - l_3^2) + m_3^2 (1 - m_3^2) + n_3^2 (1 - n_3^2) \right] \left[5 \left(\frac{1}{u_1^3} + \frac{2}{u_2^3} \right) \sum_0 \right. \right.$$
$$+ \left(\frac{3}{u_1^5} + \frac{2}{u_2^5} \right) \left(\frac{2\mu_N H}{\hbar} a \right)^2 \sum_1 + 2 \left(\frac{1}{u_1^5} + \frac{4}{u_2^5} \right) \left(\frac{2\mu_N H}{\hbar} a \right)^2 \sum_2 \left. \right]$$
$$\left. + 4 (l_3^2 m_3^2 + m_3^2 n_3^2 + n_3^2 l_3^2) \left(\frac{-1}{u_1^5} + \frac{1}{u_2^5} \right) \left(\frac{2\mu_N H}{\hbar} a \right)^2 \sum_3 \right\} . \qquad (58)$$

Since the corresponding transition probability to the reverse process of the spin-Umklappung mentioned above is clearly seen to become $W_d \exp(-2\mu_N H/kT) \approx W_d$ except for the extremely low temperatures, we have, for the nuclear spin-lattice relaxation time T_1 due to the direct process in the polycrystalline solids,*

$$T_1^{-1} = \frac{27}{5} \frac{a^3}{\pi\hbar^6} (\mu_N \mu_e)^2 (2\mu_N H) \frac{m^2}{M} \left(\frac{E_p - E_s}{E_p - E_s + a_2 - a_1} \right)^4 R^2 \frac{\exp(2\mu_N H/kT)}{\exp(2\mu_N H/kT) - 1}$$
$$\times \left\{ 2 \left(\frac{1}{u_1^3} + \frac{2}{u_2^3} \right) \cdot \sum_0 + \frac{2}{5} \left(\frac{3}{u_1^5} + \frac{2}{u_2^5} \right) \left(\frac{2\mu_N H}{\hbar} a \right)^2 \sum_1 + \frac{4}{5} \left(\frac{1}{u_1^5} + \frac{4}{u_2^5} \right) \right.$$
$$\left. \times \left(\frac{2\mu_N H}{\hbar} a \right)^2 \sum_2 + \frac{4}{5} \left(\frac{-1}{u_1^5} + \frac{1}{u_2^5} \right) \left(\frac{2\mu_N H}{\hbar} a \right)^2 \sum_3 \right\} , \qquad (59)$$

on account of the relations $\langle l_3^2 (1 - l_3^2) + m_3^2 (1 - m_3^2) + n_3^2 (1 - n_3^2) \rangle_{AV} = 2/5$ and $\langle l_3^2 m_3^2 + m_3^2 n_3^2 + n_3^2 l_3^2 \rangle_{AV} = 1/5$.

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* As clearly seen in (58), the transition probability due to the direct process of nuclear spin-Umklappung appears to become zero in case of an external magnetic field directed along one of the principal axes of the crystal ($l_3 = 1$, $m_3 = n_3 = 0$, etc.), which leads to infinitely large relaxation times in contradistinction to the experimental observations. Such situation, however, is not so surprising, because the approximate expressions of the matrix elements described in (42) are responsible for such unfavourable results; which are easily observed to be removed by proceeding, to a higher approximation, the evaluations of the concerned matrix elements or by refining the crystal model in our case in accordance with experimental observations. In order to estimate the order of magnitude of T_1 for the polycrystalline solids, however, we shall be allowed to adopt the expression of (59).

§ 5. Numerical results and comparison with experiments

In order to estimate the order of magnitudes of T_1, we have to evaluate the integrals of R, K and J, in which the explicit specifications of the electronic energy band structure in the crystalline solids are required. For that purpose, we shall assume tentatively for the highest filled band and the lowest unfilled one to be $3s$- and $3p$-bands respectively. The radial eigenfunctions of the corresponding atomic orbitals may be written as

$$R_{3s}(r)=a_H^{-2}(2(Z-s)/3a_H)^{7/2}/\sqrt{6!}\cdot(r/a_H)^2\exp(-(Z-s)r/3a_H) \qquad (60\cdot1)$$

and

$$R_{3p}(r)=a_H^{-2}(2(Z-s')/3a_H)^{7/2}/\sqrt{6!}\cdot(r/a_H)^2\exp(-(Z-s')r/3a_H) \qquad (60\cdot2)$$

by the use of Slater's method of shielding constant,[11] in which the best fitted analytical functions to the numerical data of Hartree's self-consistent field method have been worked in accordance with the experimental results. Ze is the nuclear charge, s and s' the screening constants for $3s$ and $3p$ electrons respectively, a_H the Bohr orbit.

By use of $(60\cdot1)$ and $(60\cdot2)$, the integral R is easily evaluated as follows.

$$R=\sqrt{3}\cdot896\,a_H[(Z-s)(Z-s')/(2Z-s-s')^2]^{7/2}/(2Z-s-s'),$$

$$\therefore\quad R^2=0.675\cdot10^{-10}[(Z-s)(Z-s')/(2Z-s-s')^2]^7/(2Z-s-s')^2. \qquad (61)$$

Similarly, we are able to evaluate both integrals of J and K, which results have been described in the Appendix on account of the rather lengthy expression.

Furthermore, the following appropriate values of the various physical quantities involved in (59) have been provisionally adopted for the numerical estimates of the spin-lattice relaxation time for the polycrystalline solids.

$a=2.5\cdot10^{-8}$ cm, $\hbar=1.0541\cdot10^{-27}$ erg·sec (Birge's recent value),
$\mu_e=0.93\cdot10^{-20}$ erg·gauss^{-1}, $\mu_N\sim2.4\cdot10^{-23}$ erg·gauss^{-1},
$m=9.1\cdot10^{-28}$ g, $M\sim4.04\cdot10^{-23}$ g, $Z=12$,
$u_1\sim2.5\cdot10^5$ cm·sec^{-1}, $H=10^4$ gauss,
$\Delta E\sim10$ ev, $\beta_2\sim\gamma_2\sim3$ ev,
$\delta_1=u_1/u_2$, $\delta=(E_p-E_s)/(E_p-E_s+u_2-u_1)\sim(1-(u_2-u_1)/(E_p-E_s))\lesssim1$.

Using the abbreviations mentioned above, our formula for the nuclear spin-lattice relaxation time T_1 becomes, for $2\mu_NH\ll kT$,

$$T_1^{-1}=\frac{27}{5}\frac{a^3}{\pi\hbar^6}(\mu_N\mu_e)^2\frac{m^2}{M}R^2\delta^4kT\Big\{2(1+2\delta_1^3)/u_1^3\cdot\sum\nolimits_0+2(3+2\delta_1^5)/5u_1^5$$
$$\times\Big(\frac{2\mu_NH}{\hbar}a\Big)^2\sum\nolimits_1+4(1+4\delta_1^5)/5u_1^5\cdot\Big(\frac{2\mu_NH}{\hbar}a\Big)\sum\nolimits_2+4(\delta_1^5-1)/5u_1^5$$
$$\times\Big(\frac{2\mu_NH}{\hbar}a\Big)^2\cdot\sum\nolimits_3\Big\}, \qquad (62)$$

from which the following numerical results for T_1 have been obtained.

Table 1. Numerical Values of R, J and K

$s=9.15$, $s'=11$	$R=0.46\cdot10^{-16}$	$J=-0.49\cdot10^{28}$	$K=-0.54\cdot10^{22}$
$s=s'=9.15$	$R=1.63\cdot10^{-14}$	$J=-2.84\cdot10^{25}$	$K=1.08\cdot10^{26}$

Table 2. Numerical Values of T_1

	$s=9.15$, $s'=11$	$s=s'=9.15$
$\delta_1=1.4$	$0.5_5/T$ sec	$6.5/T$ sec
$\delta_1=2.0$	$0.1_1/T$ sec	$1.1/T$ sec

The case of $s=s'=9.15$ means the partial shielding for $3p$ electron, corresponding to an isolated atom in accordance with Slater's rule, while the case of $s=9.15$ and $s'=11$ represents the complete shielding for $3p$ electrons, the latter of which seems to be more favourable for the electrons within the crystals from the theoretical viewpoint. These two cases, however, have been worked numerically to clarify the effect upon T_1 of the crystal electron binding to each ion within the crystal.

Thus, the order of magnitude of T_1 according to our formula are observed to become of about $10^{-1}\sim10$ sec near the temperature $T\sim1°K$. The close examination of our formula, however, reveals that the mentioned order of magnitude of T_1 depends strongly upon the various physical quantities characteristic for the crystalline solids under consideration, i. e., the sound velocity, the electronic band structure (β_1, β_2, γ_2), the corresponding eigenfunctions, etc., and, thus, it appears to vary rather widely through the small changes of the mentioned quantities, i. e., by a factor of about 10^2 or 10^{-2} compared with the above mentioned numerical estimates at low temperatures according to the various kinds of crystalline solids. On the other hand, the nuclear spin-lattice relaxation time is observed experimentally to range between 10^{-4} and 10^2 seconds at very low temperatures, i. e., $T_1=280$ sec ($T=1.2°K$), 67 sec ($T=4.2°K$) for the nucleus of F^{19} in CaF_2, or $T_1=5$ sec ($T_1=2°K$) for the nucleus of Li^7 in LiF or $T_1=10\sim10^{-2}$ sec ($T=1°\sim10°K$) for the proton in $CaAl(SO_4)_2\cdot12H_2O$ and so on. Our numerical estimates of T_1 are clearly seen to be qualitative agreements with the experimental observations in view of the various simplifications regarding the electronic band structures and the approximations involved in the concerned matrix elements. In this connection, it should be stressed that the remarkably short but favourable relaxation times in our theory, compared with that of Waller's one, have resulted from the relatively large interactions of $\delta\mathfrak{H}_{eI}$ and $\delta\mathfrak{H}_{eN}$ together with taking account of all the contributions of crystal electrons within the $3s$-band.

The variations of the relaxation time T_1 with both the external field H and the temperature T shall be discussed in detail in Part II since the observed variations of T_1 with the mentioned quantities are considered to be ascribed to both processes of Direct and Raman types as shown in (19).

Furthermore, it should be remarked that Bloembergen's mechanism of spin diffusion to paramagnetic impurities involved or Pound's mechanism due to quadrupole moment in nuclei may be considered, for some specified crystalline solids, to be superimposed upon our relaxation mechanism described above, in which case the rather complicated behaviours

of T_1 with H and T will be considered probably to appear but the radical modifications in the order of magnitude of T_1 are not expected in such case in view of the relaxation times due to each of the mentioned three mechanisms being shown to be roughly of equal order of magnitude.

In view of the mentioned situations, therefore, our proposed mechanism for the nuclear spin-lattice relaxation in the crystalline solids may be concluded to go on a right direction in elucidating the still completely unsettled phenomena of the nuclear magnetic relaxation in solids. The further refinement of our general theory proposed here will be highly required owing to the circumstance that the nuclear magnetic relaxation in solids is one of the most interesting but still unsolved problems in such field.

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Appendix

$$J=1/\sqrt{3}\cdot\int_0^\infty d\rho\int_{-\infty}^{\infty}dz\,R_s(\sqrt{\rho^2+z^2})\,R_p(\sqrt{\rho^2+(z-a)^2})\,\frac{\rho(z-a)(2z^2-\rho^2)}{(\rho^2+z^2)^{5/2}(\rho^2+(z-a)^2)^{1/2}},$$

$$K=1/\sqrt{3}\cdot\int_0^\infty d\rho\int_{-\infty}^{\infty}dz\,R_s(\sqrt{\rho^2+(z-a)^2})\,R_p(\sqrt{\rho^2+z^2})\,\frac{\rho z(2z^2-\rho^2)}{(\rho^2+z^2)^3}.$$

On performing the change of variables ρ and z into r and r', i. e.,

$$r^2=\rho^2+z^2,\quad r'^2=\rho^2+(z-a)^2,$$

with

$$\rho d\rho dz=rr'/a\cdot dr\,dr',$$

it follows

$$J=1/8\sqrt{3}\,a^4\cdot\left\{\int_0^a dr\int_{a-r}^{a+r}dr'+\int_a^\infty dr\int_{r-a}^{r+a}dr'\right\}R_s(r)\,R_p(r')\,rr'(r^2-r'^2-a^2)$$
$$\times\{3(r^2-r'^2+a^2)^2-4a^2r^2\}/r^4$$

and

$$K=1/8\sqrt{3}\,a^4\cdot\left\{\int_0^a dr\int_{a-r}^{a+r}dr'+\int_a^\infty dr\int_{r-a}^{r+a}dr'\right\}R_s(r')\,R_p(r)\,r'(r^2-r'^2+a^2)$$
$$\times\{3(r^2-r'^2+a^2)^2-4a^2r^2\}/r^5.$$

Substituting (60·1) and (60·2) into the above integrals, we get, after a rather lengthy but elementary calculation, the following results.

The case of $s\neq s'$: $(Z_s=(Z-s)/3a_H,\ Z_p=(Z-s')/3a_H)$.

$$J=\frac{1}{45\sqrt{3}\,a^3}(Z_sa)^{7/2}(Z_pa)^{5/2}\left\{\exp(-Z_sa)\cdot\left(1152+\frac{36000}{(Z_pa)^2}+\frac{241920}{(Z_pa)^4}\right)/(Z_pa)^3\right.$$
$$\left.+\exp(-Z_sa)\cdot\left\{\left(\frac{48}{Z_pa}+\frac{528}{(Z_pa)^2}+\frac{3312}{(Z_pa)^3}+\frac{14304}{(Z_pa)^4}+\frac{40320}{(Z_pa)^5}+\frac{54000}{(Z_pa)^6}\right)/(Z_sa-Z_pa)\right.\right.$$

$$-\left(\frac{48}{Z_p a}+\frac{512}{(Z_p a)^2}+\frac{2928}{(Z_p a)^3}+\frac{9648}{(Z_p a)^4}+\frac{13680}{(Z_p a)^5}\right)/(Z_s a-Z_p a)^2+\left(\frac{160}{Z_p a}+\frac{1024}{(Z_p a)^2}\right.$$
$$\left.+\frac{3168}{(Z_p a)^3}+\frac{4032}{(Z_p a)^4}\right)/(Z_s a-Z_p a)^3-\left(96+\frac{384}{Z_p a}+\frac{864}{(Z_p a)^2}+\frac{864}{(Z_p a)^3}\right)/(Z_s a-Z_p a)^4\}$$
$$-\exp(-Z_p a)\cdot\left\{\left(16+\frac{240}{Z_p a}+\frac{1696}{(Z_p a)^2}+\frac{7968}{(Z_p a)^3}+\frac{25968}{(Z_p a)^4}+\frac{54000}{(Z_p a)^5}+\frac{54000}{(Z_p a)^6}\right)/(Z_s a\right.$$
$$-Z_p a)-\left(48+\frac{400}{Z_p a}+\frac{1968}{(Z_p a)^2}+\frac{6528}{(Z_p a)^3}+\frac{13680}{(Z_p a)^4}+\frac{13680}{(Z_p a)^5}\right)/(Z_s a-Z_p a)^2+\left(96\right.$$
$$\left.+\frac{544}{Z_p a}+\frac{1888}{(Z_p a)^2}+\frac{4032}{(Z_p a)^3}+\frac{4032}{(Z_p a)^4}\right)/(Z_s a-Z_p a)^3-\left(96+\frac{384}{Z_p a}+\frac{864}{(Z_p a)^2}\right.$$
$$\left.+\frac{864}{(Z_p a)^3}\right)/(Z_s a-Z_p a)^4\}+\exp(-Z_s a)\cdot\left\{\frac{48}{Z_p a}-\frac{528}{(Z_p a)^2}+\frac{3312}{(Z_p a)^3}-\frac{14304}{(Z_p a)^4}+\frac{40320}{(Z_p a)^5}\right.$$
$$\left.-\frac{54000}{(Z_p a)^6}\right)/(Z_s a+Z_p a)-\left(\frac{48}{Z_p a}-\frac{512}{(Z_p a)^2}+\frac{2928}{(Z_p a)^3}-\frac{9648}{(Z_p a)^4}+\frac{13680}{(Z_p a)^5}\right)/(Z_s a+Z_p a)^2$$
$$+\left(\frac{160}{Z_p a}-\frac{1024}{(Z_p a)^2}+\frac{3168}{(Z_p a)^3}-\frac{4032}{(Z_p a)^4}\right)/(Z_s a+Z_p a)^3+\left(96-\frac{384}{Z_p a}+\frac{864}{(Z_p a)^2}\right.$$
$$\left.-\frac{864}{(Z_p a)^3}\right)/(Z_s a+Z_p a)^4\}+\exp(-Z_p a)\cdot\left\{\left(16+\frac{240}{Z_p a}+\frac{1696}{(Z_p a)^2}+\frac{7968}{(Z_p a)^3}+\frac{25968}{(Z_p a)^4}\right.\right.$$
$$\left.\left.+\frac{54000}{(Z_p a)^5}+\frac{54000}{(Z_p a)^6}\right)/(Z_s a+Z_p a)+\left(48+\frac{400}{Z_p a}+\frac{1968}{(Z_p a)^2}+\frac{6528}{(Z_p a)^3}+\frac{13680}{(Z_p a)^4}\right.\right.$$
$$\left.\left.+\frac{13680}{(Z_p a)^5}\right)/(Z_s a+Z_p a)^2+\left(96+\frac{544}{Z_p a}+\frac{1888}{(Z_p a)^2}+\frac{4032}{(Z_p a)^3}+\frac{4032}{(Z_p a)^4}\right)/(Z_s a+Z_p a)^3\right.$$
$$\left.+\left(96+\frac{384}{Z_p a}+\frac{864}{(Z_p a)^2}+\frac{864}{(Z_p a)^3}\right)/(Z_s a+Z_p a)^4\right\}-\exp(-Z_p a)\cdot\left\{\frac{96}{Z_p a}+\frac{1152}{(Z_p a)^2}\right.$$
$$\left.+\frac{7776}{(Z_p a)^3}+\frac{36000}{(Z_p a)^4}+\frac{116640}{(Z_p a)^5}+\frac{241920}{(Z_p a)^6}+\frac{241920}{(Z_p a)^7}\right\}+\exp(-Z_p a)\left\{48+\frac{576}{Z_p a}+\frac{3888}{(Z_p a)^2}\right.$$
$$\left.+\frac{18000}{(Z_p a)^3}+\frac{58320}{(Z_p a)^4}+\frac{120960}{(Z_p a)^5}+\frac{241920}{(Z_p a)^6}+\frac{241920}{(Z_p a)^7}\right\}+\exp(-Z_p a)\cdot Z_s a/(Z_p a)^2$$
$$\times\left\{48+\frac{576}{Z_p a}+\frac{3888}{(Z_p a)^2}+\frac{18000}{(Z_p a)^3}+\frac{58320}{(Z_p a)^4}+\frac{120960}{(Z_p a)^5}+\frac{120960}{(Z_p a)^6}\right\}\cdot E_i(-Z_s a+Z_p a)$$
$$-\exp(+Z_p a)\cdot Z_s a/(Z_p a)^2\cdot\left\{48-\frac{576}{Z_p a}+\frac{3888}{(Z_p a)^2}-\frac{18000}{(Z_p a)^3}+\frac{58320}{(Z_p a)^4}-\frac{120960}{(Z_p a)^5}\right.$$
$$\left.+\frac{120960}{(Z_p a)^6}\right\}\cdot E_i(-Z_s a-Z_p a)\Big\},$$

$$E_i(x)=\int_{\infty}^{-x}\exp(-u)/u\cdot du\,.$$

$$K=\frac{1}{45\cdot\sqrt{3}\,a^3}(Z_s a)^{5/2}(Z_p a)^{7/2}\Big\{-\exp(-Z_p a)\left\{\left(2592+\frac{136080}{(Z_s a)^2}+\frac{1088640}{(Z_s a)^4}\right)\right.$$

$$\times (Z_p a-1)/(Z_s a)^4+\left(144+\frac{23760}{(Z_s a)^2}+\frac{498960}{(Z_s a)^4}+\frac{1088640}{(Z_s a)^6}\right)/(Z_s a)^2\Big\}-\exp(-Z_p a)$$

$$\times\left\{\left(\frac{64}{Z_s a}+\frac{1024}{(Z_s a)^2}+\frac{8448}{(Z_s a)^3}+\frac{40992}{(Z_s a)^4}+\frac{112320}{(Z_s a)^5}+\frac{136080}{(Z_s a)^6}\right)/(Z_p a-Z_s a)-\left(\frac{64}{Z_s a}\right.\right.$$

$$+\frac{976}{(Z_s a)^2}+\frac{6048}{(Z_s a)^3}+\frac{18576}{(Z_s a)^4}+\frac{23760}{(Z_s a)^5}\Big)/(Z_p a-Z_s a)^2+\left(\frac{224}{Z_s a}+\frac{1472}{(Z_s a)^2}+\frac{4320}{(Z_s a)^3}\right.$$

$$\left.+\frac{5184}{(Z_s a)^4}\right)/(Z_p a-Z_s a)^3-\left(96+\frac{384}{Z_s a}+\frac{864}{(Z_s a)^2}+\frac{864}{(Z_s a)^3}\right)/(Z_p a-Z_s a)^4+\exp(-Z_s a)$$

$$\times\left\{\left(16+\frac{304}{Z_s a}+\frac{2880}{(Z_s a)^2}+\frac{16800}{(Z_s a)^3}+\frac{62160}{(Z_s a)^4}+\frac{136080}{(Z_s a)^5}+\frac{136080}{(Z_s a)^6}\right)/(Z_p a-Z_s a)\right.$$

$$-\left(48+\frac{480}{Z_s a}+\frac{2880}{(Z_s a)^2}+\frac{10800}{(Z_s a)^3}+\frac{23760}{(Z_s a)^4}+\frac{23760}{Z(_s a)^5}\right)/(Z_p a-Z_s a)^3+\left(96+\frac{604}{Z_s a}\right.$$

$$+\frac{2336}{(Z_s a)^2}+\frac{5184}{(Z_s a)^3}+\frac{5184}{(Z_s a)^4}\Big)/(Z_p a-Z_s a)^3-\left(96+\frac{384}{Z_s a}+\frac{864}{(Z_s a)^2}\right.$$

$$\left.+\frac{864}{(Z_s a)^3}\right)/(Z_p a-Z_s a)^4\Big\}+\exp(-Z_p a)\left\{\frac{64}{Z_s a}-\frac{1024}{(Z_s a)^2}+\frac{8448}{(Z_s a)^3}-\frac{40992}{(Z_s a)^4}+\frac{112320}{(Z_s a)^5}\right.$$

$$-\frac{136080}{(Z_s a)^6}\Big)/(Z_p a+Z_s a)-\left(\frac{64}{Z_s a}-\frac{976}{(Z_s a)^2}+\frac{6048}{(Z_s a)^3}-\frac{18576}{(Z_s a)^4}+\frac{23760}{(Z_s a)^5}\right)/(Z_p a+Z_s a)^2$$

$$+\left(\frac{224}{Z_s a}-\frac{1472}{(Z_s a)^2}+\frac{4320}{(Z_s a)^3}-\frac{5184}{(Z_s a)^4}\right)/(Z_p a+Z_s a)^3+\left(96-\frac{384}{Z_s a}+\frac{864}{(Z_s a)^2}\right.$$

$$\left.-\frac{864}{(Z_s a)^3}\right)/(Z_p a+Z_s a)^4\Big\}+\exp(-Z_s a)\left\{\left(16+\frac{304}{Z_s a}+\frac{2880}{(Z_s a)^2}+\frac{16800}{(Z_s a)^3}+\frac{62160}{(Z_s a)^4}\right.\right.$$

$$+\frac{136080}{(Z_s a)^5}+\frac{136080}{(Z_s a)^6}\Big)/(Z_p a+Z_s a)+\left(48+\frac{480}{Z_s a}+\frac{2880}{(Z_s a)^2}+\frac{10800}{(Z_s a)^3}+\frac{23760}{(Z_s a)^4}\right.$$

$$+\frac{23760}{(Z_s a)^5}\Big)/(Z_p a+Z_s a)^2+\left(96+\frac{604}{Z_s a}+\frac{2336}{(Z_s a)^2}+\frac{5184}{(Z_s a)^3}+\frac{5184}{(Z_s a)^4}\right)/(Z_p a+Z_s a)^3$$

$$+\left(96+\frac{384}{Z_s a}+\frac{864}{(Z_s a)^2}+\frac{864}{(Z_s a)^3}\right)/(Z_p a+Z_s a)^4\Big\}+\exp(-Z_s a)\left\{144+\frac{2592}{Z_s a}\right.$$

$$\left.+\frac{23760}{(Z_s a)^2}+\frac{136080}{(Z_s a)^3}+\frac{498960}{(Z_s a)^4}+\frac{1088640}{(Z_s a)^5}+\frac{1088640}{(Z_s a)^6}\right\}\cdot Z_p a/(Z_s a)^2-\exp(-Z_s a)$$

$$\times\left\{\left(72+\frac{1296}{Z_s a}+\frac{11880}{(Z_s a)^2}+\frac{68040}{(Z_s a)^3}+\frac{249480}{(Z_s a^4)}+\frac{544320}{(Z_s a)^5}+\frac{544320}{(Z_s a)^6}\right)((Z_p a)^2\right.$$

$$-(Z_s a)^2)/(Z_s a)^3+\left(64+\frac{1168}{Z_s a}+\frac{10800}{(Z_s a)^2}+\frac{62160}{(Z_s a)^3}+\frac{228480}{(Z_s a)^4}+\frac{498960}{(Z_s a)^5}\right.$$

$$\left.+\frac{498960}{(Z_s a)^6}\right)/Z_s a\cdot E_i(-Z_p a+Z_s a)\Big\}+\exp(Z_s a)\left\{\left(\frac{64}{Z_s a}-\frac{1168}{(Z_s a)^2}+\frac{10800}{(Z_s a)^3}-\frac{62160}{(Z_s a)^4}\right.\right.$$

$$+\frac{228480}{(Z_s a)^5}-\frac{498960}{(Z_s a)^6}+\frac{498960}{(Z_s a)^7}\Big)+\left(72-\frac{1296}{Z_s a}+\frac{11880}{(Z_s a)^2}-\frac{68040}{(Z_s a)^3}+\frac{249480}{(Z_s a)^4}\right.$$

$$-\frac{544320}{(Z_s a)^5}+\frac{544320}{(Z_s a)^6}\Big)\{((Z_p a)^2-(Z_s a)^2)/(Z_s a)^3\}E_i(-Z_p a-Z_s a)\Big\}\,.$$

The case of $s=s'$:

$$J=\frac{1}{\sqrt{3}\cdot 45a^3}(Z_s a)^6\Big\{-\exp(-Z_s a)\Big(4+\frac{106\cdot 7}{Z_s a}+\frac{1715\cdot 2}{(Z_s a)^2}+\frac{9035\cdot 8}{(Z_s a)^3}+\frac{39190}{(Z_s a)^4}+\frac{87297}{(Z_s a)^5}$$
$$+\frac{172099}{(Z_s a)^6}-\frac{69820}{(Z_s a)^7}\Big)-\exp(Z_s a)E_i(-2Z_s a)\Big(\frac{48}{Z_s a}-\frac{576}{(Z_s a)^2}+\frac{3888}{(Z_s a)^3}-\frac{18000}{(Z_s a)^4}$$
$$+\frac{58320}{(Z_s a)^5}-\frac{120960}{(Z_s a)^6}+\frac{120960}{(Z_s a)^7}\Big)\Big\}\,.$$

$$K=\frac{1}{\sqrt{3}\cdot 45a^3}(Z_s a)^6\Big\{\exp(-Z_s a)\Big(4+\frac{264\cdot 4}{Z_s a}+\frac{3764\cdot 1}{(Z_s a)^2}+\frac{33076}{(Z_s a)^3}+\frac{143916}{(Z_s a)^4}+\frac{366862}{(Z_s a)^5}$$
$$+\frac{709912}{(Z_s a)^6}-\frac{288008}{(Z_s a)^7}\Big)+\exp(Z_s a)E_i(-2Z_s a)\Big(\frac{64}{Z_s a}-\frac{1168}{(Z_s a)^2}+\frac{10800}{(Z_s a)^3}-\frac{62160}{(Z_s a)^4}$$
$$+\frac{228480}{(Z_s a)^5}-\frac{498760}{(Z_s a)^6}+\frac{498760}{(Z_s a)^7}\Big)\Big\}\,.$$

References

1) Bloembergen, Purcell and Pound, Phys. Rev. **73** (1948), 679.
Bloembergen, Physica **15** (1949), 386.
Hatton and Rollin, Nature **160** (1947), 436; Phys. Rev. **74** (1948), 346; Proc. Roy. Soc. A**199** (1949), 222.
2) Waller, ZS. f. Phys. **79** (1936), 152.
Heitler and Teller, Proc. Roy. Soc. A**149** (1936), 152.
Fierz, Physica **5** (1938), 433.
3) Bloembergen *et al*, loc. cit.
Gutowsky, Kistiakowsky, Pake and Purcell, J. Chem. Phys. **17** (1949), 972.
Gutowsky and Pake, ibid. **18** (1950), 162.
Newman. ibid. **18** (1950), 669.
Sachs, Thesis, Harvard University (1950).
Turner, Thesis, Harvard University (1950).
4) Heitler and Teller, loc. cit.
5) Bloembergen, Physica **15** (1949), 588.
6) Bloembergen, ibid. **15** (1949), 386.
7) Pound, Phys. Rev. **79** (1950), 685.
8) Waller, loc. cit.
Van Vleck, Phys. Rev. **57** (1940), 426.
9) Wilson, Proc. Roy. Soc. A**133** (1931), 458; A**134** (1931), 277.
10) Waller, loc. cit.
11) Seitz, *Modern Theory of Solids* (1940).
12) Bloembergen, Purcell and Pound, loc. cit.
13) Wilson, loc. cit.
14) Slater, Phys. Rev. **36** (1930), 57.

Letters to the Editor

Note on the Saturation Properties of Nuclear Forces

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In a previous letter[1] to the Editor of the Physical Review, one of the authors has concluded that in a heavy nucleus the ordinary part of nuclear forces V_{ord} vanishes if we take account of the exclusion principle, but this conclusion is not correct. H. Miyazawa pointed out to us that when two nucleons exchange the mesons of zero momentum the exclusion principle need not to be taken into account, i.e. in this case we must put $(1-f(p_1))(1-f(p_2))=1$ instead of zero, and $\bar{V}_{ord}$ does not vanish.

Further, T. Kinoshita and H. Miyazawa[2] found a possibility to account for the saturation properties of nuclear forces in the following way: the mass of mesons in a heavy nucleus is different from that in a free space, and the difference is proportional to P^3 after the Fermi gas model of nuclei, where P is the maximum momentum of the Fermi gas. The binding energy per nucleon W is given by

$$-W=\frac{3P^2}{10M}+\alpha P^3\int J(r)dv+\beta X,$$

where α is a constant which depends on the exchange character of the nuclear force and βX is the exchange term. If we make use of $J(r)=\frac{e^{-\mu r}}{r}$, we get $4\pi\alpha\frac{P^3}{\mu^2}$ for the ordinary term; as μ is equal to μ_0+ const. $\times P^3$, $\frac{P^3}{\mu^2}$ has a maximum. Employing the Serber potential, Kinoshita and Miyazawa showed that the binding energy per nucleon is equal to 5 Mev if we put $\delta\mu=35\left(\frac{P}{P_0}\right)^3$, where P_0 is the value of P obtained by taking the nuclear radius equal to the experimental value and is about 210 Mev.

In order to verify the saturation properties of nuclear forces, we must furthermore show that both the spin-parallel nucleus and the neutron cluster are unstable or at least metastable. We have calculated these binding energies per nucleon by employing the following forms of nuclear potential;

$$\text{(I)}\quad V_{NP}=V_{PP}=V_{NN}=-\frac{g^2}{4\pi}\cdot\frac{1-P_\sigma P_\tau}{2}\cdot\frac{e^{-\mu r}}{r},\left(\frac{g^2}{4\pi}=0.479\right),$$

$$\text{(II)}\quad V_{NP}=-\frac{g_0^2}{4\pi}\frac{1-P_\sigma P_\tau}{2}\frac{e^{-\mu r}}{r},\left(\frac{g_0^2}{4\pi}=0.479\right),$$

$$V_{PP}=V_{NN}=\frac{g_1^2}{2\pi}\frac{1}{\mu^2}(\sigma_1 d)(\sigma_2 d)\frac{e^{-\mu r}}{r},\left(\frac{g_1^2}{4\pi}=0.0209\right).$$

The result is as follows:

$$\text{(I)}\quad -W=\frac{3P^2}{10M}-\frac{g^2}{8\pi}\cdot\left[f(P,\mu)+\frac{9}{16\pi}g(P,\mu)\right],\ \text{for standard nuclei.}$$

$$-W=\frac{3P^2}{10M}-\frac{g^2}{8\pi}\cdot\left[f(P,\mu)+\frac{3}{16\pi}g(P,\mu)\right],\ \text{for spin-parallel nuclei and neutron clusters.}$$

$$f(P,\mu)=\frac{P^3}{\pi\mu^2},$$

$$g(P,\mu)=4P-\frac{2\mu^2}{3P}+\left(\frac{2\mu^2}{P}+\frac{\mu^4}{6P^3}\right)\cdot l_n\frac{4P^2+\mu^2}{\mu^2}-\frac{16\mu}{3}\tan^{-1}\frac{2P}{\mu}.$$

When we put $\delta\mu=40\left(\frac{P}{P_0}\right)^3$, W for standard nuclei has a maximum at $P=P_0$, and $W_{max}\approx 12.2$ Mev. W for spin-parallel nuclei and neutron clusters has a maximum at $P=140$ Mev, and $W_{max}\approx -0.9$Mev. So we might conclude that these nuclei are unstable.

$$\text{(II)}\quad -W=\frac{3P^2}{10M}-\frac{g_0^2}{8\pi}\frac{2}{3}f(P,\mu)$$

$$-\left(\frac{g_0^2}{8\pi}+\frac{g_1^2}{4\pi}\right)\cdot\frac{3}{8\pi}g(P,\mu),\quad \text{for standard nuclei,}$$

$$-W=\frac{3P^2}{10M}-\left(\frac{g_0^2}{8\pi}-\frac{g_1^2}{6\pi}\right)\frac{1}{3}f(P,\mu)$$

$$-\left(\frac{g_0^2}{8\pi}+\frac{g_1^2}{6\pi}\right)\frac{3}{16\pi}g(P,\mu),\quad \text{for spin-parallel nuclei,}$$

$$-W=\frac{3P^2}{10M}-\frac{g_1^2}{6\pi}\frac{9}{16\pi}g(P,\mu),\quad \text{for neutron clusters.}$$

When we put $\delta\mu=49\left(\frac{P}{P_0}\right)^3$, W for standard nuclei has a maximum at $P=P_0$, and $W_{max}\approx 5.7$ Mev. Also in this case W's for spin-parallel nuclei and neutron clusters are negative. We can safely assure that the former is unstable or metastable even after taking into account the approximation of the Fermi gas model and the latter is unstable.

Our conclusion is that the saturation properties of nuclear forces are comprehensible considering the change of mass of mesons in a heavy nuclei.

The authors wish to thank Mr. H. Miyazawa for valuable and helpful suggestions which he gave about this calculation.

1) H. Kanazawa, Phys. Rev. **86** (1952), 428(L).
2) T. Kinoshita and H. Miyazawa, Private communication.

A Note on the S-Matrix in the Theory of the Non-local Interaction

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We can define S-matrix in the theory of the non-local interaction either by the formal integration of the field equations after the method of Källén[1] and Yang-Feldman[2], or by the extension of the chronological operator of Dyson modifying after the investigations of Matthews[3] and Koba.[4] (Hereafter the modified operator is denoted by P^* after Koba.) But the above two S-matrices can easily be shown to be equivalent in the actual computation.

By the method of Yang-Feldman, Rayski[5]* has recently calculated the S-matrix for the electromagnetic and spinor fields with non-local interaction. Independently Shono-Oda[6]** have investigated the same problem and derived the S-matrix with the P^*-symbol. Their results differ in the electron self-energy, though in the other points they coincide. It is our purpose to examine the origin of the discrepancy between them

For brevity's sake, we discuss in details only one type of non-local interaction which is discussed by Rayski in § 1 of A and also by Shono-Oda in § 2 of B. The S-matrix in B is given by P^*-symbol as follows,

$$S=\sum_{n=0}^{\infty}\frac{(i)^n}{n}\int_{-\infty}^{+\infty}\cdots\int[dx][dx'] \cdot P^*(L'(x_1,x_1')\cdots,L'(x_n,x_n')), \qquad (1)$$

$$L'(x,x')=j_\mu(x)\eta(x-x')A_\mu(x'),$$

where $\eta(x)$ is the regularization function which is denoted by $F(x)$ in Rayski's paper. The expression of the electron self-energy derived from (1) by Shono-Oda is

$$\delta m\psi(x)=-\frac{ie^2}{4}\int\gamma_\mu S_F(x-x')\cdot D_F^{RR}(x-x')\gamma_\mu\psi(x')(dx'), \qquad (2)$$

and that derived by Rayski is

$$\delta m\psi(x)=-\frac{e^2}{2}\int\gamma_\mu[S^{(1)}(x-x')\cdot\bar{D}^{RR}(x-x')+\bar{S}(x-x')D^{(1)}(x-x')]\gamma_\mu\psi(x')(dx'). \qquad (3)$$

Concerning this expression, Rayski says that the electron self-energy is divergent because the second

* Hereafter we refer this paper as A.
** Hereafter we refer this paper as B.

term in (3) is left unchanged and diverges. However, these terms should not be integrated separately, but it must be united together and parametrized in a suitable form. For this purpose, it will be most natural to adopt the method of parametrization used successfully in the local theory.

Using the relation

$$F(o)=1 \text{ and } \bar{D}^{RR}(x)=-\frac{1}{(2\pi)^4}\cdot P\int\frac{F^2(k^2)}{k^2}\exp(ikx)(dk), \qquad (4)$$

the integrand of eq. (3) is parametrized in the momentum space as follows,

$$\begin{aligned}&\frac{\delta((p-k)^2+m^2)}{k^2}F^2(k^2)+\frac{\delta(k^2)}{(p-k)^2+m^2}\\&=\left\{\frac{\delta((p-k)^2+m^2)}{k^2}+\frac{\delta(k^2)}{(p-k)^2+m^2}\right\}\\&\quad\times F^2(k^2)\\&=-\int_0^1 dy\ \delta'[k^2(1-y)\\&\quad+((p-k)^2+m^2)y]F^2(k^2), \qquad (5)\end{aligned}$$

where $F(k^2)$ is the Fourier transform of the regularization function and in the actual evaluation we may take the form of $F(k^2)$ as

$$F^2(k^2)=\lambda^2/(k^2+\lambda^2). \qquad (6)$$

Then, introducing the well-known translation of the origin $k_\mu\to k_\mu+f_\mu y$ and observing the relation

$$\int(dk)\,\delta^{(n)}(k^2+A)g(k^2)=Re\int_{C_F}(dk)\frac{g(k^2)}{(k^2+A)^{n+1}}\cdot\frac{(-1)^n n!}{i\pi}, \qquad (7)$$

Eq. (3) is reduced to

$$\delta m\psi(x)=\frac{2ie^2}{(2\pi)^8}\int_0^1 dy\,Re\int(dk)\cdot(i\gamma k+i\gamma py-m)F^2(k+py)(k^2+m^2y^2)^{-2}\cdot\int(dp)\psi(p)\exp(ipx). \qquad (3')$$

On the other hand, with the aid of the integral representation of Feynman

$$F^2(k^2)/k^2(k'^2+m^2)=\int_0^1 dy[k^2(1-y)+(k'^2+m^2)y]^{-2}F^2(k^2), \qquad (8)$$

and the relation

$$D_F^{RR}(x)=\frac{-2i}{(2\pi)^4}\cdot\lim_{\varepsilon\to+0}\int(dk)\frac{F^2(k^2)}{k^2-i\varepsilon}\exp(ikx),$$

and making the translation of the origin in the same manner as the above, eq. (2) can be reduced to

$$\delta m\psi(x)=\frac{2ie^2}{(2\pi)^8}\int_0^1 dy\int(dk)(i\gamma k+i\gamma py-m)F^2(k+py)(k^2+m^2y^2)^{-2}\cdot\int(dp)\psi(p)\exp(ipx). \qquad (2')$$

Thus we can immediately infer that Eqs. (2) and (3) are identical. If we take such regularization factor as reference(6), Eqs. (2) and (3) do of course converge, which is against Rayski's conjection. (But the footnote in page 1293 of Rayski's paper might mean implicitly this circumstance.)

The above discussion can also be applied to the case of another type of non-local interaction discussed by Rayski in § 2 of A and also by Shono-Oda in § 4 of B. And it can be easily shown that their expressions of electron self-energy both coincide and converge against Rayski's conjection.

The author wishes to express his sincere thanks to Prof. K. Sakuma and Mr. N. Shono for their useful discussions.

1) G. Källén, Arkiv for Fysik **2** (1950), 371.
2) C. N. Yang and D. Feldman, Phys. Rev. **79** (1950), 972.
3) P. T. Matthews, Phys. Rev. **76** (1949), 684; Phil. Mag. **41** (1950), 185.
4) Z. Koba, Prog. Theor. Phys. **5** (1950), 696.
5) J. Rayski, Phil. Mag. **42** (1951), 1289.
6) N. Shono and N. Oda, Prog. Theor. Phys. (to be published.)

Note on the Structure of the Interactions between Unstable Elementary Particles

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Indeed the appearance of many unstable particles makes us imagine there are some sorts of regularties among the mass spectra of elementary particles[1]. Under this situation attempts to select and classify the interactions between so called Megalomorphs should be pursued. Such an approach was recently proposed by Pais[2]. Here we treat these problems in a little more general way. As is shown typically by decay modes, every elementary particles seem to be connected with each other by direct and indirect couplings. At present, two sorts of stable matters are known, namely nucleons and light stable particles (electrons, neutrino, γ-ray and possibly μ^0-meson). Here we may tentatively assume that no stable particles heavier than nucleon exist. The natural decays the interactions between parent and daugnter particles. Starting from known particles, we can assign each unstable particle a number λ which defines the mode of interactions with nucleon and lighter stable particles. Thanks to β-decay ($n\to p+e+\nu$), μ-decay ($\mu\to e+\nu(\mu^0)+\nu(\mu^0)$) and π-decay ($\pi\to\mu+\nu(\mu^0)$) we can deduce successively the following interactions phenomenologically

$$\begin{pmatrix} e \\ \mu \\ \pi \end{pmatrix} \rightleftarrows (N+\bar{N}) + \textit{light stable particles} + (\nu \textit{ or } \mu^0),$$

where N denotes nucleon and $\bar{N}$ anti-nucleon. We write the coupling

$A^*B^*C^*\cdots\cdots LMN+C.C.$ as

$$L+M+N+\cdots\cdots \rightleftarrows A+B+C+\cdots.$$

As regards the couplings between photon and charged particles we treat them as usual[3]. Then if we know the decay schemes, we can deduce the following types of coupling between unstable particle A and nucleons and lighter stable particles

$$A \rightleftarrows m \text{ particle nucleon} + n \text{ anti-particle nucleon} + \text{lighter stable particles.} \qquad (1)$$

We assign a number $\lambda=m-n$ to A as $A(\lambda)$. Even when we cannot identify all decay products, if we adopt a possible λ for unknown particle, we have the possible λ for parent particle. Next we consider the most general interactions such as $A(\lambda_a)^*B(\lambda_b)^*C(\lambda_c)^*\cdots\cdots L(\lambda_l)M(\lambda_m)N(\lambda_n)\cdots\cdots$ where $A,B,C,\cdots L,M,N,\cdots\cdots$ are *Bosons* and *Fermions*, and this interaction is assumed to satisfy every conditions for elementary interactions. In these interactions only the cases where

$$-(\lambda_a+\lambda_b+\lambda_c+\cdots)+(\lambda_l+\lambda_m+\lambda_n+\cdots)=0, \qquad (2)$$

are allowed, because otherwise the *conservation of nucleons* cannot be assured and the stability of matter will ultimately be destroyed by this interaction. From the scheme (1) we see that those particles lighter than nucleon should have $\lambda=0$. It should be noted that the λ-value does not relate a priori to the spin of that particle. For instance, both decay schemes $A^\circ\to p+\pi^-$ and $B^\circ\to p+\mu^-$ lead to $\lambda=1$ but A° and B° have different statistics. In the latter case $N\bar{N}B^\circ$ coupling is forbidden according to the rule (2). Moreover, there may be particles with $\lambda=0$ which are heavier than nucleon. That is, if $C^\circ\to\chi^+\chi^-$ can occur then C° have $\lambda=0$ and is heavier than nucleon ($m_\chi\sim 1200 m_e$). In general we cannot exclude the possible existence of the particles with $|\lambda|>2$, though our present knowledge tempts us to deny such possibilities. As an application of our rule, we briefly treat here the problems of newly-found heavy particles.[4] As regards V°, v° and τ-mesons, they were discussed thoroughly by many authors[5]. Here we also comprise χ-mesons[6]. Most probable decays are $V^\circ\to p+\pi^-$ (or $p+\mu^-+\nu$). $v^\circ\to\pi^++\pi^-$ (or $\pi^++\pi^-+\gamma$) and $\chi\to\mu+2\nu$ (or $e+2\nu$). We don't consider the possible existence of short-lived parents of these particles. Then hitherto known Megalomorphs are divided into

1) *The nucleon family* ($\lambda=1$)
   No (1) (nucleons), N_1 (1) (V°-meson)
2) *π-meson family* ($\lambda=0$). Strong coupling with nucleon family. $\Pi_0(0)$ (π-meson), $\Pi_1(0)$ (v°-meson), $\Pi_n(0)$ (χ-meson), γ-ray.
3) *Electron family* ($\lambda=0$). Weak coupling with nucleon and π-meson family and their mere

decay products, μ-meson, electron, neutrino, possibly μ^0-meson.

From the above assumed decay scheme, χ becomes Fermion but belongs to π-group. If the short-lived parent of χ exists, χ can be a mere decay product and may be attributed to electron family. But we are not sure same families have the same statistics. There remains the possibility that the classification with λ is a first step and each group have various statistics as an fine structure. As regards the χ-decay, it is remarkable that a universal interaction with the same coupling constant among all spin $\frac{1}{2}$ particles leads to consistent life times of χ-decay (10^{-9} *sec.*). Next, we consider all possible coupling between nucleon and π-meson families. For brevity, we confine ourselves to the couplings of the type $A_i(\lambda_a)B_j(\lambda_b)C_k(\lambda_c)$. From selection rule (2) and Pais's *even-odd rules*

$$\begin{aligned} &\lambda_a+\lambda_b+\lambda_c\neq 0 \quad \textit{Forbidden} \\ &i+j+k=\textit{even} \quad \textit{strong} \quad (G^2 \quad 1), \quad (3) \\ &i+j+k=\textit{odd} \quad \textit{odd} \quad (g^2\sim 10^{11}), \end{aligned}$$

the only allowed couplings involving χ-meson are $\bar{\Pi}_n(0)\ \Pi_n(0)\Pi_0(0)$ (*strong*) and $\bar{\Pi}_n(0)\Pi_n(0)\Pi_1(0)$ (*weak*). That is $\bar{\Pi}_n(0)\ \Pi_n(0)\ \Pi_1(0)$ is so weak that the decay $\Pi_1(0)\to\Pi_0(0)+\pi_0(0)$ via $\Pi_n(0)\Pi_n(0)\ \Pi_0(0)$ have a long life time ($10^{-9}\sim 10^{-10}$ *sec.*). As χ appears in pairs in these couplings the value of n remains unsettled. The only couplings responsible for χ-production are $\bar{\Pi}_n(0)\ \Pi_n(0)\ \Pi_0(0)$ and χ may be produced in pairs as,

$$\begin{aligned} &N+N\to N+N+\chi+\bar{\chi}, \\ &\textit{through} \quad \bar{N}_0N_0\Pi_0 \quad \textit{and} \quad \bar{\Pi}_n\Pi_n\Pi_0 \\ &N+\pi\to N+\chi+\bar{\chi}. \end{aligned}$$

Threshold energies of incident nucleon and π-meson in laboratory system are about *3.2 Bev.* and *1.7 Bev.*, respectively. Of course, the pairwise production should be checked in experiments. More comprehensive and general study along these lines is in progress.

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1) Y. Nambu, private communication.
2) A. Pais, "On the V-particles" to be published. The author wishes to express his thanks to Dr. A. Pais for sending his manuscript before publication.
3) This shows that $\lambda=1$ for nucleon.
4) Especially, see the reports of Bristol and Rochester Conference. The author is indebted to Dr. C. C. Butler for the communication of his results.
5) For the treatment along the lines here adopted, see Y. Nambu *et. al.*, Prog. Theor. Phys. **6** (1951), 615, 619; S. Oneda, ibid. **6** (1951), 633, 1014.
6) C. O'Ceallaigh, Phil. Mag. **42** (1951), 1032; R.B. Leighton and S. D. Wanlass, Phys. Rev. **86** (1952), 426. See also the reference (4).

Isotopic Spin of Nucleons and Leptons and Anti-particle Coordinate

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Owing to the existence of anti-particles, nucleons and leptons have three charge states, $+e$, $-e$, and 0. It seems, therefore, to be unsatisfactory to consider nucleons and leptons to be particles with isotopic spin $\frac{1}{2}$ [1]. In this article, however, we show that this is not the case and we can assign $\frac{1}{2}$ to the isotopic spin of nucleons and leptons.

Because the formulations are the same for nucleons and leptons, we consider in the following only the lepton case. We denote electron and neutrino fields by ψ_e and ψ_ν respectively, and lepton field by eight component spinor Ψ, which has the form

$$\Psi=\begin{bmatrix}\psi_e\\ \psi_\nu\end{bmatrix},$$

$$\text{so that} \quad \tau_3\begin{bmatrix}\psi_e\\ 0\end{bmatrix}=\begin{bmatrix}\psi_e\\ 0\end{bmatrix} \text{ and } \tau_3\begin{bmatrix}0\\ \psi_\nu\end{bmatrix}=-\begin{bmatrix}0\\ \psi_\nu\end{bmatrix}. \quad (1)$$

We expand Ψ in the form

$$\Psi(x)=\sum_{\boldsymbol{K}}\left\{A^{(1)}_{\boldsymbol{K}}\begin{bmatrix}u^{(1)}_{\boldsymbol{K}}\\ 0\end{bmatrix}+A^{(i)}_{\boldsymbol{K}}\begin{bmatrix}u^{(1)}_{\boldsymbol{K}}\\ 0\end{bmatrix}\right.$$

$$\left.+B^{*(2)}_{-\boldsymbol{K}}\begin{bmatrix}v^{(1)}_{\boldsymbol{K}}\\ 0\end{bmatrix}+B^{*(1)}_{-\boldsymbol{K}}\begin{bmatrix}v^{(1)}_{\boldsymbol{K}}\\ 0\end{bmatrix}+a^{(1)}_{\boldsymbol{K}}\begin{bmatrix}0\\ u^{(1)}_{\boldsymbol{K}}\end{bmatrix}\right.$$

$$+a_{\boldsymbol{K}}^{(2)}\begin{bmatrix}0\\ u_{\boldsymbol{K}}^{(2)}\end{bmatrix}+b_{-\boldsymbol{K}}^{*(2)}\begin{bmatrix}0\\ \tau' {}_{\boldsymbol{K}}^{(1)}\end{bmatrix}+b_{-\boldsymbol{K}}^{*(1)}\begin{bmatrix}0\\ \tau' {}_{\boldsymbol{K}}^{(2)}\end{bmatrix}\Big\},\quad(2)$$

where $u_{\boldsymbol{K}}^{(i)}(\boldsymbol{x})$ and $v_{\boldsymbol{K}}^{(i)}(\boldsymbol{x})$ are four component spinors and form a complete set of normalized orthogonal eigenfunctions of Dirac Hamiltonian $\alpha\frac{1}{i}\frac{\partial}{\partial \boldsymbol{x}}+\beta m$. They satisfy[2]

$$\frac{1}{i}\frac{\partial}{\partial \boldsymbol{x}}u_{\boldsymbol{K}}^{(i)}(\boldsymbol{x})=\boldsymbol{K}u_{\boldsymbol{K}}^{(i)}(\boldsymbol{x}),$$

$$\frac{1}{i}\frac{\partial}{\partial \boldsymbol{x}}v_{\boldsymbol{K}}^{(i)}(\boldsymbol{x})=\boldsymbol{K}v_{\boldsymbol{K}}^{(i)}(\boldsymbol{x}),\quad(3)$$

$$\Big(\alpha\frac{1}{i}\frac{\partial}{\partial \boldsymbol{x}}+\beta m\Big)u_{\boldsymbol{K}}^{(i)}(\boldsymbol{x})=(m^2+\boldsymbol{K}^2)^{\frac{1}{2}}u_{\boldsymbol{K}}^{(i)}(\boldsymbol{x}),$$

$$\Big(\alpha\frac{1}{i}\frac{\partial}{\partial \boldsymbol{x}}+\beta m\Big)v_{\boldsymbol{K}}^{(i)}(\boldsymbol{x})=-(m^2+\boldsymbol{K}^2)^{\frac{1}{2}}v_{\boldsymbol{K}}^{(i)}(\boldsymbol{x}),\quad(4)$$

and further if $\boldsymbol{K}$ is parallel or antiparallel to z-axis, they satisfy

$$\begin{aligned}&\sigma_z u_{\boldsymbol{K}}^{(1)}(\boldsymbol{x})=+u_{\boldsymbol{K}}^{(1)}(\boldsymbol{x}),\\ &\sigma_z v_{\boldsymbol{K}}^{(1)}(\boldsymbol{x})=+v_{\boldsymbol{K}}^{(1)}(\boldsymbol{x}),\\ &\sigma_z u_{\boldsymbol{K}}^{(2)}(\boldsymbol{x})=-u_{\boldsymbol{K}}^{(2)}(\boldsymbol{x}),\\ &\sigma_z v_{\boldsymbol{K}}^{(2)}(\boldsymbol{x})=-v_{\boldsymbol{K}}^{(2)}(\boldsymbol{x}).\end{aligned}\quad(5)$$

The commutation relations between $A_{\boldsymbol{K}}^{(i)}, B_{\boldsymbol{K}}^{(i)}, a_{\boldsymbol{K}}^{(i)}$, and $b_{\boldsymbol{K}}^{(i)}$ are

$$\begin{aligned}&\{A_{\boldsymbol{K}}^{(i)*}, A_{\boldsymbol{K}'}^{(j)}\}=\{B_{\boldsymbol{K}}^{(i)*}, B_{\boldsymbol{K}'}^{(j)}\}=\{a_{\boldsymbol{K}}^{(i)*}, a_{\boldsymbol{K}'}^{(i)}\}\\ &\{b_{\boldsymbol{K}}^{(i)*}, b_{\boldsymbol{K}'}^{(j)}\}=\delta_{ij}\delta_{\boldsymbol{K}\boldsymbol{K}'},\end{aligned}\quad(6)$$

corresponding to

$$\{\Psi_\sigma^*(\boldsymbol{x}),\ \Psi_{\sigma'}(\boldsymbol{x}')\}=\delta_{\sigma\sigma'}\delta(\boldsymbol{x}-\boldsymbol{x}').\quad(7)$$

Upon introducing occupation number operators

$$\begin{aligned}&N_{\boldsymbol{K}}^{(i)}=A_{\boldsymbol{K}}^{(i)*}A_{\boldsymbol{K}}^{(i)},\quad \bar{N}_{\boldsymbol{K}}^{(i)}=B_{\boldsymbol{K}}^{(i)*}B_{\boldsymbol{K}}^{(i)},\\ &n_{\boldsymbol{K}}^{(i)}=a_{\boldsymbol{K}}^{(i)*}a_{\boldsymbol{K}}^{(i)},\quad \bar{n}_{\boldsymbol{K}}^{(i)}=b_{\boldsymbol{K}}^{(i)*}b_{\boldsymbol{K}}^{(i)},\end{aligned}\quad(8)$$

the total energy and momentum of the field are given by

$$\begin{aligned}&\int\Psi^*(\boldsymbol{x})\Big(\alpha\frac{1}{i}\frac{\partial}{\partial \boldsymbol{x}}+\beta\frac{1+\tau_3}{2}m_e+\beta\frac{1-\tau_3}{2}m_\nu\Big)\Psi(\boldsymbol{x})\,dv\\ &=\sum_{\boldsymbol{K}}k_0^{(e)}(N_{\boldsymbol{K}}^{(1)}+N_{\boldsymbol{K}}^{(2)}+\bar{N}_{\boldsymbol{K}}^{(1)}+\bar{N}_{\boldsymbol{K}}^{(2)}-2)\\ &+\sum_{\boldsymbol{K}}k_0^{(\nu)}(n_{\boldsymbol{K}}^{(1)}+n_{\boldsymbol{K}}^{(2)}+\bar{n}_{-\boldsymbol{K}}^{(1)}+\bar{n}_{-\boldsymbol{K}}^{(2)}-2),\end{aligned}\quad(9)$$

where $k_0^{(e)}=(m_e^2+\boldsymbol{K}^2)^{\frac{1}{2}}$ and

$$k_0^{(\nu)}=(m_\nu{}^2+\boldsymbol{K}^2)^{\frac{1}{2}},$$

and

$$\begin{aligned}&\int\Psi^*(\boldsymbol{x})\frac{1}{i}\frac{\partial}{\partial \boldsymbol{x}}\Psi(\boldsymbol{x})\,dv\\ &=\sum_{\boldsymbol{K}}\boldsymbol{K}(N_{\boldsymbol{K}}^{(1)}+N_{\boldsymbol{K}}^{(2)}-\bar{N}_{-\boldsymbol{K}}^{(1)}-\bar{N}_{-\boldsymbol{K}}^{(2)})\\ &+\sum_{\boldsymbol{K}}\boldsymbol{K}(n_{\boldsymbol{K}}^{(1)}+n_{\boldsymbol{K}}^{(2)}-\bar{n}_{-\boldsymbol{K}}^{(1)}-\bar{n}_{-\boldsymbol{K}}^{(2)}).\end{aligned}\quad(10)$$

When we are only concerned with the field quanta whose momenta are parallel or antiparallel to z-axis, z-component of the total spin angular momentum is given by

$$\begin{aligned}&\int\Psi^*(\boldsymbol{x})\sigma_z\Psi(\boldsymbol{x})\,dv\\ &=\sum_{\boldsymbol{K}}(N_{\boldsymbol{K}}^{(1)}-N_{\boldsymbol{K}}^{(2)}+\bar{N}_{-\boldsymbol{K}}^{(1)}-\bar{N}_{-\boldsymbol{K}}^{(2)})\\ &+\sum_{\boldsymbol{K}}(n_{\boldsymbol{K}}^{(1)}-n_{\boldsymbol{K}}^{(2)}+\bar{n}_{-\boldsymbol{K}}^{(1)}-\bar{n}_{-\boldsymbol{K}}^{(2)}).\end{aligned}\quad(11)$$

From Eqs. (9), (10), and (11), it is clear that the particles represented by the occupation number $N_{\boldsymbol{K}}^{(1)}$, for example, are electrons whose energies, momenta, and spin directions are $k_0^{(e)}$, $\boldsymbol{K}$, and parallel to z-axis respectively, and so on. Especially $N_{\boldsymbol{K}}^{(i)}$ and $\bar{n}_{\boldsymbol{K}}^{(i)}$ are occupation numbers of anti-electrons and anti-neutrinos whose energies, momenta, and spins are $k_0^{(e)}$or $k_0^{(\nu)}$, $\boldsymbol{K}$, and parallel or antiparallel to z-axis according to $i=1$ or 2. It is the purpose of this article to see how the isotopic spin and charge of these particles (especially of anti-particles) will be. For this purpose, we have only to calculate the z-component of total isotopic angular momentum and total charge in quite the same way as (9), (10), and (11), namely

$$\int\Psi^*(\boldsymbol{x})\tau_3\Psi(\boldsymbol{x})\,dv$$

$$= \sum_{K} (N_{K}^{(1)} + N_{K}^{(2)} - \bar{N}_{-K}^{(1)} - \bar{N}_{-K}^{(2)} + 2)$$

$$+ \sum_{K} (-n_{K}^{(1)} - n_{K}^{(2)} + \bar{n}_{-K}^{(1)} + \bar{n}_{-K}^{(2)} - 2), \quad (12)$$

and

$$-e \int \Psi^{*}(x) \frac{1+\tau_3}{2} \Psi(x) d\tau$$

$$= -e \sum_{K} (N_{K}^{(1)} + N_{K}^{(2)} - N_{-K}^{(1)} - N_{-K}^{(2)} + 2). \quad (13)$$

From (12) and (13), it can be said that anti-particles are in states of oppositely directed isotopic spin to the ordinary particles and anti-electrons have charges of opposite sign to electrons, while anti-neutrinos have no charges as well as neutrinos. We can say electrons and anti-neutrinos (or anti-electrons and neutrinos) are in the same isotopic spin state.

Here we must answer the question why exclusion principle does not apply to the system containing one electron and one anti-neutrino, namely why it is permissible for one electron and one anti-neutrino to occupy the same spin and momentum state at the same time.

Remembering that, *in one-electron theoretical case*, we must distinguish *positive energy state* from *negative energy one* which have the same momentum and spin direction, we must distinguish "*particles*" from their "*anti-particles*" *in positron theoretical case*. In order to describe leptons unifiedly, we must introduce another coordinate which specifies whether leptons are in "particle states" or in "anti-particle states", besides ordinary space-, τ-spin-, and spin-coordinates. We shall call these new coordinates "*anti-particle coordinates*". With respect to all of these freedoms, electrons and anti-neutrinos are subject to the exclusion principle, but not with regard to space, τ-spin, and spin freedoms only. As an example, we shall consider a positronium. Even if we do not introduce τ-spin coordinate, an electron and a positron are different from each other with respect to anti-particle coordinate. Therefore, it is permissible for a positronium to be both in ^1S and ^3S states.

1) V. Votruba and M. Lokajíček, Phys. Rev. **86** (1952), 260.
2) The system of units in which $\hbar = c = 1$ is used.

Analytical Representation of Spin

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The spin operators and their eigenfunctions are usually represented by matrices.[1] It is possible, however, to represent them analytically in several ways.[2] For instance the spin operators are assumed to be the following differential operators of the two independent variables ρ and ω,

$$S_x = \hbar \left(\cos\omega \cdot \rho \frac{\partial}{\partial \rho} - \sin\omega \frac{\partial}{\partial \omega} \right),$$

$$S_y = \hbar \left(\sin\omega \cdot \rho \frac{\partial}{\partial \rho} + \cos\omega \frac{\partial}{\partial \omega} \right), \quad (1)$$

$$S_z = \frac{\hbar}{i} \frac{\partial}{\partial \omega},$$

which operate on the analytical spin eigenfunctions

$$v_+ = \sqrt{\rho}\, e^{i\omega/2}, \quad v_- = \sqrt{\rho}\, e^{-i\omega/2}, \quad (2)$$

where ρ and ω are not any concrete angle variables[2], but only abstract coordinates of the inner freedom. Then it is easily proved that all the properties, which the Pauli spin matrices have, are reserved as follows. One obtains from (1) as the commutation relations

$$S_x S_y - S_y S_x = i\hbar S_z \qquad \text{(cycl.)} \quad (3)$$

and from (1) and (2) as the operational rules

$$S_x v'_{\pm} = \frac{\hbar}{2} v'_{\mp}, \quad S_y v'_{\pm} = \pm i \frac{\hbar}{2} v'_{\mp},$$

$$S_z v'_{\pm} = \pm \frac{\hbar}{2} v'_{\pm}, \quad (4)$$

from which it follows that

$$S_x^2 v'_{\pm} = S_y^2 v'_{\pm} = S_z^2 v'_{\pm} = \frac{\hbar^2}{4} v'_{\pm}, \quad (5)$$

$$(S_x S_y + S_y S_x) v'_{\pm} = 0. \quad \text{cycl.} \quad (6)$$

It seems that the last formula (6) can hardly be derived from other models of the rotating sphere.

Now the spin operators (1) are formally transformed into those of the angular momentum:

$$S_x=\frac{\hbar}{i}\left(\eta\frac{\partial}{\partial\zeta}-\zeta\frac{\partial}{\partial\eta}\right),$$

$$S_y=\frac{\hbar}{i}\left(\zeta\frac{\partial}{\partial\xi}-\xi\frac{\partial}{\partial\zeta}\right), \qquad (7)$$

$$S_z=\frac{\hbar}{i}\left(\xi\frac{\partial}{\partial\eta}-\eta\frac{\partial}{\partial\xi}\right),$$

where ξ, η and ζ are given by

$$\xi=\rho\sin\omega,\ \eta=-\rho\cos\omega,\ \zeta=i\rho. \qquad (8)$$

But it must be noted that ξ, η and ζ are not mutually independent but related to each other by

$$\xi^2+\eta^2+\zeta^2=0, \qquad (9)$$

which suggests us that the concept of the spin may be interpreted as an angular momentum in the complex space of zero radius.

1) W. Pauli, ZS. f. Phys. **43** (1927), 601.
2) F. Bopp und R. Haag, ZS. f Naturf. **5a** (1950), 644.
N. Rosen, Phys. Rev. **82** (1951), 621.
T. Takahashi, J. Phys. Soc. Japan **7** (1952), 307.

Anisotropy in the Antiferromagnetic MnO_2

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It was pointed out by P. W. Anderson[1] that two superstructures are possible in the antiferromagnetic crystals of a rutile type; in one structure spins at the corner sites are antiparallel to those at the body center sites, and in the other the corner lattice and the body center lattice are further divided into two antiferromagnetic sublattices. According to the neutron diffraction studies[2)3)], MnF_2 and FeF_2 belong to the superstructure of the 1st kind, and MnO_2 to that of the 2nd kind.

F. Keffer[4] has shown that the anisotropy in MnF_2 arises mainly from the magnetic dipole interactions which make the spins parallel to the c axis in the case of the 1st kind as the unit cell dimension along the c axis is considerably shorter than that along the a axis in the rutile structure. It is, however, expected that in the superstructure of the 2nd kind the magnetic dipole interactions make the direction of the spins perpendicular to the c axis since + and − spins line up alternately along this direction.

In the antiferromagnetic crystals of a rutile type forming the superstructure of the 2nd kind, the crystal lattice is divided into four sublattices, each having parallel spins. Extending the treatment by F. Keffer[4] for MnF_2 to this case, the internal field at the lattice points on each sublattice arising from the magnetic dipole interactions can be written as follows:

$$H_x(1)=\Phi_{a1}M_{1x}+\Phi_{a2}M_{2x}+\Phi_{a3}M_{3x}+\Phi_{a4}M_{4x}, \quad (1)$$

$$H_z(1)=\Phi_{c1}M_{1z}+\Phi_{c2}M_{2z}+\Phi_{c3}M_{3z}+\Phi_{c4}M_{4z}, \quad (2)$$

etc.

Here $\boldsymbol{H}(i)$ and $\boldsymbol{M}_i$ are respectively the internal field and the total magnetic moment on the i-th sublattice (1 and 2 relating to the two corner sublattices and 3 and 4 to the two body center sublattices) and Φ_{ai} and Φ_{ci} represent the following lattice sum:

$$\Phi_{ai}=-\frac{4}{N}\sum_j^{(i)}[1-3\cos^2(x,\gamma_{1j})]\gamma_{1j}^{-1}, \quad (3)$$

$$\Phi_{ci}=-\frac{4}{N}\sum_j^{(i)}[1-3\cos^2(z,\gamma_{1j})]\gamma_{1j}^{-3}, \quad (4)$$

where the summation is taken over distances between a lattice point on the 1st sublattice and its neighbors j on the i-th sublattice and $N/4$ is the number of the magnetic ions on one sublattice.

By use of the internal field (1) and (2), we obtain the difference between the parallel and perpendicular susceptibilities to the c axis above the Curie temperature as

$$\chi_{\parallel}-\chi_{\perp}=\chi_{\parallel}\chi_{\perp}\frac{1}{4}[\Phi_{c1}-\Phi_{a1}+\Phi_{c2}-\Phi_{a2}+\Phi_{c3}-\Phi_{a3}+\Phi_{c4}-\Phi_{a4}]. \quad (5)$$

Below the Curie point, we can put $\boldsymbol{M}_1=-\boldsymbol{M}_2$ and $\boldsymbol{M}_3=-\boldsymbol{M}_4$ and so the anisotropy energy F becomes as

$$F=-M^2[(\Phi_{c1}-\Phi_{a1})-(\Phi_{c2}-\Phi_{a2})](\gamma_1^2+\gamma_3^2), \qquad (6)$$

where M is a magnitude of the magnetic moment of one sublattice and γ_1 and γ_3 are respectively the direction cosines of $\boldsymbol{M}_1$ and $\boldsymbol{M}_3$ with respect to the c axis. This expression of the anisotropy energy shows that the directions of $\boldsymbol{M}_1$ and $\boldsymbol{M}_2$ are independent of these of $\boldsymbol{M}_3$ and $\boldsymbol{M}_4$.

Lattice constants of MnO_2 are $c=2.89$A and $a=4.44$ A[5]. Using these constants, the value of $\Phi_c-\Phi_a$ calculated by the Ewald-Kornfeld method[6] becomes as

$$\begin{aligned}&\Phi_{c1}-\Phi_{a1}=0.12,\\ &\Phi_{c2}-\Phi_{a2}=21.58, \qquad (7)\\ &\Phi_{c3}-\Phi_{a3}=\Phi_{c4}-\Phi_{a4}=-5.14.\end{aligned}$$

Then the difference between two principal susceptibilities above the Curie point and the anisotropy energy below the Curie point in the case of MnO_2 are given by

$$\chi_{\parallel}-\chi_{\perp}=2.86\ \chi_{\parallel}\chi_{\perp}, \qquad (5)$$

$$F=21.46\ M^2(\gamma_1^2+\gamma_3^2). \qquad (6')$$

These calculated values of $\chi_{\parallel}-\chi_{\perp}$ and F show that below the Curie point the preferred directions of the spins in MnO_2 lie in the plane perpendicular to the c axis and so the susceptibility along the c axis is larger than that along the a axis both above and below the Curie point, differing from the case of MnF_2 where $\chi_{\parallel}-\chi_{\perp}$ changes its sign about at the Curie point, provided that the other parts of the anisotropy are small compared with the magnetic dipole interaction part.

As shown by (6′), the magnetic dipole interactions give rise to no anisotropy in the plane perpendicular to the c axis. This anisotropy would be given by the part arising from the crystalline field. The anisotropy Hamiltonian per spin arising from this origin can be written as

$$DS_z^2+E(S_\xi^2-S_\eta^2), \qquad (7)$$

where ξ-and η-axes coincide with the directions of (110) and $(\bar{1}10)$ for the spins on the corner lattice sites and for the spins on the body center lattice sites ξ-and η-axes exchange their directions. Above the Curie point the 2nd term gives no anisotropy[7][4] and the 1st term would be masked by the magnetic dipole interaction part (5′)[4]. Below the Curie point, the 1st term will again be masked by (6′), but the 2nd term gives rise to the anisotropy in the plane perpendicular to the c axis. As the ξ-and η-axes for the corner spins are each orthogonal to those for the body center spins, the preferred axes of $\boldsymbol{M}_1$ and $\boldsymbol{M}_2$ are orthogonal to those of $\boldsymbol{M}_3$ and $\boldsymbol{M}_4$ and each moment takes a parallel orientation to (110) or $(\bar{1}10)$. This anisotropy in the basic plane would, however, be considerably smaller.

The susceptibility expected by the above considerations is qualitatively in agreement with the single crystal susceptibility measured by Bizette and Tsai[3]. In order to estimate the value of the critical field[7] it is necessary to calculate the constant E. However this field strength would be expected to become smaller than that of MnF_2 where the anisotropy relating to the critical field arises mainly from the magnetic dipole interactions.

Thus, as pointed out by F. Keffer[4] for MnF_2, the magnetic dipole interactions are important for the anisotropy in the antiferromagnetic substances. Also in $CuCl_2\,2H_2O$, the relation between its superstructure and the preferred direction seems to show that these interactions are primarily important for the anisotropy of this substance.

1) P. W. Anderson, Phys. Rev. **79** (1950), 705. J. H. Van Vleck, J. de Phys. et Radium **12** (1951), 262.
2) R. A. Erickson and C. G. Shull, Phys. Rev. **83** (1951), 208.
3) R. A. Erickson, Phys. Rev. **85** (1952), 745.
4) F. Keffer, Phys. Rev. (1952) to be published.
5) W. G. Wyckoff, *Crystal Structures*, Interscience Publisher, IWC., New York, (1948).
6) H. Kornfeld, ZS. f. Physik **22** (1924), 27.
7) K. Yosida, Prog. Theor. Phys. **6** (1951), 691.
8) H. Bizette, J. de Phys. et Radium **12** (1951), 161.

Comparison of Born and Heitler Expansions in a Scattering Problem

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In their analysis of the scattering by a static potential, Jost and Pais[1] indicated that the Born expansion for a nuclear potential would have no useful domain of applicability, though the series might be convergent.

As an example, these authors compared, for the case of high energy N-P scattering by a central Yukawa potential, the total cross section σ and the angular ratio $R=d\sigma(180°)/d\sigma(90°)$, obtained from the second Born approximation, with the corresponding correct values computed previously by Christian and Hart[2]. The agreement was, however, not only quite unsatisfactory but also unreasonable, since the total cross section came out to be considerably greater than the correct one.

Using the damping formalism[3][4] we have reexamined this example. The integral equation for the reaction operator $\boldsymbol{K}$ and the potential V has been solved by successive substitution method corresponding to the Born approximation. Jost and Pais[1] identified the integral equation for the scattering amplitude $\boldsymbol{R}$ and V with that for $\boldsymbol{K}$ and V. This identification is of course equivalent to the omission of the damping effect and we can use their expressions directly for our $\boldsymbol{K}$. With the approximate $\boldsymbol{K}$ so obtained, the damping integral equation was solved exactly by decomposing $\boldsymbol{R}$ and $\boldsymbol{K}$ into partial waves, thus taking into account the damping effect completely[4]. Contributions from $l \geqq 6$ to $\boldsymbol{R}$ were ignored, since they were estimated to be negligible for σ and give only a few percent correction to the ratio R.

Table 1. Total cross section for Yukawa potential.*
E_0: Energy of the incident particle in the laboratory system; σ_1 and σ_2: Total cross section in first and second approximation.

E_0(Mev)	Without damping effect (Jost and Pais)		With damping effect		Correct value (Christian and Hart)
	σ_1 (mb)	σ_2 (mb)	σ_1 (mb)	σ_2 (mb)	
40	191	378	110	153	231
90	88	140	53	66	90
180	42	56	28	33	
270	27	33	19	22	

Table 2. Angular ratio for Yukawa potential*.
$R_1=d\sigma_1(180°)/d\sigma_1(90°)$; $R_2=d\sigma_2(180°)/d\sigma_2(90°)$.

E_0(Mev)	Without damping effect (Jost and Pais)		With damping effect		Correct value (Christian and Hart)
	R_1	R_2	R_1	R_2	
40	2.2	1.8	2.3	1.9	1.26
90	5.2	4.1	5.6	4.6	3.25

*The same potential has been used here as in Sec. II (b) (even theory) of the reference 1.

Results are given in Tables 1 and 2. For comparison, the values of Jost-Pais[1] and Christian-Hart[2] are also tabulated.

Thus we may conclude that, in the high energy N-P scattering by a static potential, (1) the damping effect is really considerably large and (2) it plays an important role because it remedies the unreasonable situation which appeared in the Born approximation. But our approximation method employed here is, as

a whole, not yet very authoritative due to the lack of an appropriate method of approximation for the reaction operator $\boldsymbol{K}$.

1) R. Jost and A. Pais, Phys. Rev. **82** (1951), 840.
2) Richard S. Christian and Edward W. Hart, Phys. Rev. **77** (1950), 441.
3) Marvin L. Goldberger, Phys. Rev. **84** (1951), 929.
4) N. Fukuda, Prog. Theor. Phys. to be published. Our $\boldsymbol{K}=-\boldsymbol{G}$ of Goldberger.

Diffusion of the Nucleonic Component in the Atmosphere

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Diffusion of the nucleonic component in the atmosphere is investigated by many authors based on the hypothesis of the nucleon-cascade. One of the authors showed that in deducing the formula two kinds of the treatment are possible as in the cascade shower theory in the earlier paper. In spite of the clear physical meaning of the results the method of the successive collision is so inconvenient for the overall aspects of the diffusion that we resort to the method of the Mellin-transformation which has been developed recently in that subject by many authors[2]. In these treatments two mean free paths (m.f.p.) appear, one is the collision mean free path, and the other is the absorption m.f.p.. It is, however, assumed that the collision m.f.p. is equal to the corresponding value of the geometrical cross section and the absorption m.f.p. is equated to the experimental value. Therefore, many sorts of the theory can co-exist which give the same results and the necessity of the concept of the nucleon-cascade may not be guaranteed.

These considerations suggest that we need the more direct evidence of the nucleon-cascade theoretically and experimentally. Recent development of the emulsion technique gives the apparent evidence of the secondary high energy nucleons up to 1 Gev produced in the high energy nuclear collisions[3]. In the present note we show that the more careful treatment gives the fine structure of the diffusion of the nucleonic component such as the variation of the absorption m.f.p. with energy and atmospheric depth. These results can interpret the experiments semi-quantitatively This fact may support the nucleon-cascade hypothesis on the theoretical point of view.

For simplicity, we say only on the nucleons (protons and neutrons) and the argument of heavier nuclei is omitted. Including the latter, the circumstances are not changed so much (except for the n-p ratio)[4].

The nucleons in the atmosphere are classified as follows[5]

A-nucleons: above 1.5Gev. Their nuclear interactions are observed as showers in the emulsions or penetrating showers in the counter or cloud chamber experiments, and caused the secondary A- or B-nucleons and mesons. (One half of the 1.5 Gev nucleons colliding nuclei can produce the meson and the other half cannot.)[6]

B-nucleons: 400 Mev~1.5 Gev. Their nuclear interaction can hardly result in the meson production, but always cause the production of the secondary C-nucleons. These events are observed sometimes as showers and otherwise stars.

C-nucleons: 50 Mev~400 Mev. Their nuclear interactions cause the production of the low energy secondary nucleons which are observed as stars.

D-nucleons: below 50 Mev. They are the final products of the chain of the nuclear interactions occurring successively in the atmosphere.

Since comparatively simple model of the nucleon-cascade may be applied to A-nucleons, here we treat only the subjects concerning with these nucleons.

It is assumed that the spectrum of the secondary nucleons is of the form

$$V(E,E_0)dE=N\cdot V(E/E_0)dE/E_0, \quad (1)$$

where E_0 and E are the kinetic energies of the incident and the secondary nucleon, respectively, and N, the number of the emitted nucleons, is of the order 2, which corresponds to the survivals of the incident and the recoil nucleons in the nucleus.

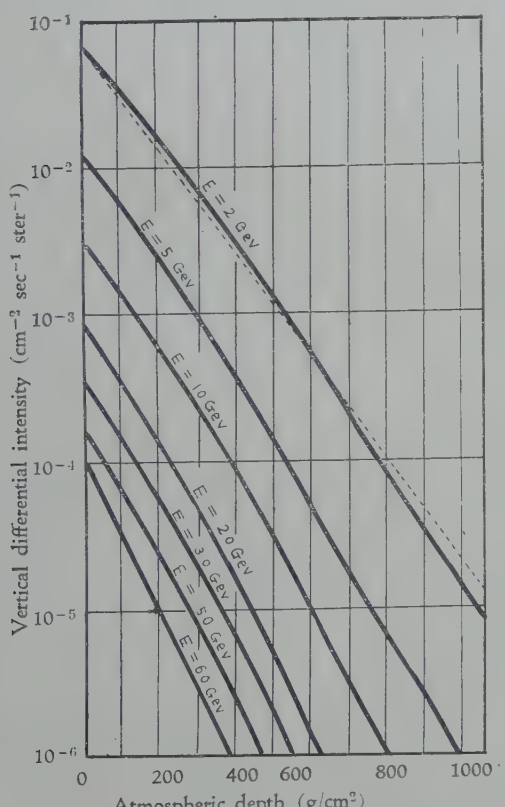
Simple calculation shows that the altitude dependence of the nucleonic component with the primary spectrum of the form $aE^{-(\gamma+1)}$ is approximately represented as

$$aE^{-(\gamma+1)}\exp\left[-\left\{1-V(\gamma+1)\right\}x\right], \quad (2)$$
$$V(\gamma+1)=\int_0^1 s^\gamma V(s)\,ds,$$

Now, the primary spectrum of the nucleonic component has the knee at about 60 Gev. Above this energy the power γ is assumed to be 1.8 and below this energy 0.9.[7] Experiment gives the absorption m.f.p. of the burst producing nucleons with secondaries with the total energy 60 Gev to be approximately geometrical.[8] This fact, combining the above discussion suggests that

$$1-V(2.8)\simeq 65/70. \qquad (3)$$

The value 65 g/cm^2 corresponds to the geometrical cross section and 70 g/cm^2 is obtained from the barometric effect of the burst frequencies by Stinchcomb. Nextly, the absorption m.f.p. of the penetrating showers detected by the counter trays, of which agents have mainly from several Gev up to a few ten Gev energies, is about 120g/cm^2.[9] In that energy region the power of the primary spectrum is 0.9 and therefore,



The slop of the dotted line corresponds to 120 g/cm^2, and that of the line with energy 60 Gev to 80 g/cm^2.

$$1-V(1.9)\simeq 65/120. \qquad (4)$$

(3) and (4) give some restrictions to the spectrum of the secondary, i.e. the form of the $V(E,E_0)$.

Precise calculation gives the following results:

(a) Absorption m.f.p. is gradually elongated with decreasing energy of the nucleons, from nearly the geometrical value to the experimentally observed value on the penetrating showers.

(b) For the energy slightly above the geomagnetic cut off energy, the slope of the attenuation curve is steeper above tha mountain altitude than below,[10] where it becomes almost equal to the amount defined by (4). (Strictly speaking, calculated value is by a few percent shorter than 120 g/cm^2.)

(c) For the nucleons with energy slightly below the knee, the attenuation near the top of the atmosphere is decided by (4). The deeper the atmosphere, the steeper the slope of the attenuation curve becomes, and finally the slope reaches the value corresponding the geometrical cross section.

The figure shows the typical case where we choose Heitler-Janossy spectrum as $V(E,E_0)$ and N is taken to be 1.65. Then 1-V(2.8) and 1-V(1.9) correspond to the absorption m.f.p. of 80 g/cm^2 and 120 g/cm^2 respectively. We find this choice of N gives slightly shorter m.f.p. for the low energy nucleons than the experimental value.

Thus the simple model of the nucleon-cascade here adopted seems to be able to interpret the diffusion of the nucleonic component to the considerable extent. The full paper including the comprehensive discussion with respect to B- and C-nucleons, primary heavier nuclei and n-p ratio will be reported in this journal.

In conclusion the authors should like to express their sincere thanks to Prof. T. Inoue for his continued encouragement, and Prof. S. Hayakawa for his valuable discussions.

1) H. Kita and H. Hasegawa, Prog. Theor. Phys. **4** (1949), 376(L).
2) For example, H. Messel, Phys. Rev. **83** (1951), 21.
3) U. Camerini, J. H. Davies, P. H. Fowler, C. Franzinetti, W. O. Lock, D. H. Perkins and G. Yukutieti, Phil. Mag. **42** (1951), 1241.
4) K. Sakihama and S. Takagi, Prog. Theor. Phys. **6** (1951), 1017 (L).
5) S. Hayakawa, Kagaku **22** (1952), 278. (in Japanese).

We had classified as follows:
A-nucleons: Above 2 Gev, B-nucleons: 400 Mev~2 Gev, C-nucleons: 60~400 Mev, D-nucleons; below 60 Mev.

However Hayakawa's classification has been published and is essentially not so much different from ours that we use his classification.

6) U. Camerini et al. loc. cit.
7) J. R. Winkler, T. Stix, K. Dwight and R. Sabin, Phys. Rev. **79**(1950), 656.
8) T. G. Stinchcomb, Phys. Rev. **83**(1951), 422; T. Kameda and M. Wada, Prog. Theor. Phys. **7**(1952) 1.
9) B. Rossi, Rev. Mod. Phys. **20** (1948), 537.
10) T. Kameda and M. Wada, loc. cit.

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A New Attempt on the Self-Energy Problem of the Photon

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The self-energy problem of the photon is investigated using an idea of renormalizing the light velocity. It is shown in § 2 and § 3 that the self-energy ΔE and the alteration of the light velocity due to the interaction Δc are connected by the relation

$$E+\Delta E=p(c+\Delta c),$$

where E, p, and c are the energy, the momentum, and the velocity of a free photon respectively. In § 4 c is renormalized on the ground of this relation, and a theory of the interaction of the electromagnetic and electron fields is given in a form which is invariant under Lorentz and a gauge transformation, and is free from the divergence of the self-energy of the photon. § 5 is devoted to the description of the Lagrangian formalism of the theory. Calculations in this paper are restricted to the e^2 approximation.

§ 1. Introduction

The divergence of the self-energy of the photon has been a dead-lock in quantum electrodynamics and many attempts have been done to overcome this difficulty. But none of them seem to have gained a final success. These attempts, including Schwinger's[1] theory, Pauli-Villars'[2] regulator, or Umezawa et al.[3] -Feldman's[4] mixed fields, are all aiming at to annulate the self-energy terms. Are they, however, the only ways in this problem? We want to propose in this paper another one based on quite a different idea of renormalizing the light velocity.

Let us begin the discussion with a re-examination of Einstein's classical work on the theory of relativity. In his theory the vacuum was considered as a medium to transmit electromagnetic waves, and, accordingly, the propagation velocity of the light in vacuum appeared as an important natural constant to determine the structure of the space-time. After the accomplishment, however, the theory of relativity seems to have been considered too formally. Although it is on one hand a framework of all physical laws, we believe that the content of this theory also can not stand apart from the evolutions of our recognition about the nature. Thus it would be a reasonable conjecture to expect that a profound reform brought about by the introduction of the quantum theory must permeate into the theory of relativity. Consider, for example, the interaction of the electromagnetic field with the electron field. The vacuum is then defined according to Dirac's positron theory as a state in which all negative energy states are occupied. This state is, however, nothing but a sort of Fermi gas at the absolute zero of temperature, and it may be expected that the refraction index of the vacuum deviates from unity and so the propagation

velocity of the light is altered from that of no interaction. Here we must point out that what Einstein used as a signal in his theory corresponds to the light in this Fermi gas, or, in other words, the photon "*clothed*" with virtual electro-positron pairs, so that the constant c appearing in Lorentz-transformation must be regarded as the velocity of this clothed photon. This means that Lorentz-transformation, and, therefore, the structure of the space time is altered as a result of the interaction, and that it would be necessary in the investigation of the self-energy problem of the photon to take into account this situation.

The rest mass of a particle is determined from its energy and momentum by the relation ;

$$E^2=p^2c^2+\mu^2c^4. \tag{1·1}$$

Therefore

$$E=pc \tag{1·2}$$

is the condition that the particle should have a vanishing rest mass. As to the photon, (1·2) is of course satisfied if there is no interaction. When interactions with charged fields are introduced, the self-energy terms appear and (1·2) seems to be violated. It should be noted, however, that c is also altered as a result of the interaction, for, the advent of c in (1·1) or in (1·2) is through Lorentz-transformation, and c appearing there was the velocity of the clothed photon. Hence the photon will be observed to have a vanishing rest mass even when we take into account the contribution from the self-energy terms, if the alterations of E and c satisfy

$$E+\Delta E=p(c+\Delta c).* \tag{1·3}$$

This is because in the actual world Lorentz transformation should be constructed using $c+\Delta c$ instead of unobservable c. The self-energy terms will be ignored in such a situation if we replace c by $c+\Delta c$, and the contradiction to the invariance of gauge will disappear. Thus we can hope to use for our problem the renormalization technique proposed by Tomonaga[5] and Schwinger[1] just as in the case of the self-energy problem of the electron. Writing the Hamiltonian of the electromagnetic field as a function of c in the form

$$H(c)=H(c+\Delta c)-\frac{\partial H}{\partial c}\Delta c,$$

we replace $c+\Delta c$ by the observed value of c, c_{ob}, and treat $H(c_{ob})$ as a Hamiltonian of the free clothed photon, while $\partial H/\partial c\cdot\Delta c$ will serve as a new counter term to cancel divergent effects produced by ordinary interactions. In this way we shall be able to reach to a theory of the interaction of the electromagnetic and electron fields which is free from the pathological divergence of the self-energy of the photon without endeavouring to annulate the self-energy terms.

It is the purpose of the present paper to discuss the possibility of this program. We calculate in § 2 and § 3 the alterations of the energy, the momentum, and the velocity of

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* Alteration of p may be conceivable. But as will be seen in § 3, Δp vanishes at least in the e^2 approximation, and therefore we disregarded it from the beginning to simplify the discussion.

a photon due to the interaction with the electron field, and it is shown in the beginning of § 4 that (1·3) is satisfied at least in the e^2 approximation. In the remainder of § 4 we develop a renormalization procedure outlined above. It is found in the course of the process, however, that we can not follow Tomonaga or Schwinger's idea literally. The cause is the mathematical ambiguities contained in the calculations of ΔE or of Δc, and it becomes necessary to admit that the counter term in our theory could not be canceled exactly by replacing c by c_{ob} in the Hamiltonian of the free clothed photon. Thus our theory might result in the introduction of a new interaction, and it is required to confirm whether such an interaction can be taken into the theory consistently. This is done in § 5, where a Lagrangian formalism of the theory is given employing a quantization procedure proposed by Kanesawa and Koba.[7] Concerning the contributions to ΔE or to Δc from charged fields other than the electron field, or the self-energy problem of those fields of vanishing mechanical rest mass other than the electromagnetic field which could be used equally as signals in Einstein's theory, we give only a brief discussion in the concluding remarks of § 6.

§ 2. The velocity of a clothed photon

The velocity of a particle is usually calculated from its energy and momentum using

$$p/E=v/c^2.$$

This relation can not be used in our case, since, calling in question Lorentz transformation itself, we do not know the right value of c. Therefore let us calculate it directly from the equation of motion of the field which describes the clothed photon.

It would be convenient to give here a general description of the formalism which will be used in this paper. In order to make the gauge invariance explicit, we adopt the one in which the electromagnetic field is decomposed into the transverse, longitudinal, and scalar components. The decomposition can be conveniently expressed by introducing an arbitrary time-like unit vector n_μ as

$$A_\mu(x)=n_\mu dA(x)-(\partial/\partial x_\mu+n_\mu d)A'(x)+\mathfrak{A}_\mu(x)\,. \tag{2·1}$$

$A(x)$, $A'(x)$, and $\mathfrak{A}_\mu(x)$ are operators which satisfy the equations of motion

$$\begin{aligned}&\Box A(x)=0\,,\\ &\Box A'(x)=0\,,\\ &\Box \mathfrak{A}_\mu(x)=0\,,\end{aligned} \tag{2·2}$$

and the commutation relations

$$\begin{aligned}&[A(x),\,A(x')]=i\hbar c\,\mathfrak{D}(x-x'),\\ &[A'(x),\,A'(x')]=-i\hbar c\,\mathfrak{D}(x-x'),\\ &[\mathfrak{A}_\mu(x),\,\mathfrak{A}_\nu(x')]=i\hbar c\,\delta_{\mu\nu}D(x-x')+i\hbar c\,n_\mu n_\nu D(x-x')\\ &\qquad -i\hbar c(\partial/\partial x_\mu+n_\mu d)(\partial/\partial x_\nu+n_\nu d)\,\mathfrak{D}(x-x'),\end{aligned} \tag{2·3}$$

where $\mathfrak{D}(x)$ is defined by

$$d^2\mathfrak{D}(x)=D(x), \tag{2·4}$$

and $$\Box\mathfrak{D}(x)=0,$$

and we used an abbreviation

$$d=(n_\lambda\partial/\partial x_\lambda).$$

$\mathfrak{A}_\mu(x)$ satisfies further

$$n_\mu\mathfrak{A}_\mu(x)=0, \quad \partial\mathfrak{A}_\lambda(x)/\partial x_\mu=0. \tag{2·5}$$

Under the gauge transformation

$$A_\mu(x)\to A_\mu(x)+\partial_\mu\lambda(x), \tag{2·6}$$
$$\Box\lambda(x)=0,$$

$\Lambda(x)$, $\Lambda'(x)$, and $\mathfrak{A}_\mu(x)$ transform as

$$\begin{aligned}&\Lambda(x)\to\Lambda(x)-\lambda(x),\\ &\Lambda'(x)\to\Lambda'(x)-\lambda(x),\\ &\mathfrak{A}_\mu(x)\to\mathfrak{A}_\mu(x).\end{aligned} \tag{2·7}$$

Therefore $(\Lambda(x)-\Lambda'(x))$ and $\mathfrak{A}_\mu(x)$ remain gauge invariant, and the gauge invariance of the theory is made explicit if we can express all physical quantities with $(\Lambda(x)-\Lambda'(x))$ and $\mathfrak{A}_\mu(x)$ only.

With a subsidiary condition imposed on the state vector $\Psi[\sigma]$

$$(\Lambda(x)-\Lambda'(x))\Psi[\sigma]=0, \tag{2·8}$$

the Schrödinger equation is given by

$$i\hbar c\frac{\delta\Psi[\sigma]}{\delta\sigma(x)}=(H_1(x)+H_2(x))\Psi[\sigma], \tag{2·9}$$

with

$$H_1(x)=-\frac{1}{c}j_\mu(x)\mathfrak{A}_\mu(x), \tag{2·10}$$

and

$$H_2(x)=-\int_\sigma\left(\frac{1}{2}\frac{\partial\mathfrak{D}(x-x')}{\partial x_\mu}+n_\mu d\,\mathfrak{D}(x-x')\right)\frac{1}{c}j_\mu(x)\frac{1}{c}j_\lambda(x')d\sigma_\lambda',$$

while the energy-momentum four vector is expressed as

$$P_\nu[\sigma]=P_\nu^{(0)}[\sigma]+P_\nu^{(1)}[\sigma]+P_\nu^{(2)}[\sigma], \tag{2·11}$$

with

$$\begin{aligned}P_\nu^{(0)}[\sigma]=&\frac{1}{2c}\int_\sigma d\sigma_\mu\left[\frac{\partial\mathfrak{A}_\lambda(x)}{\partial x_\mu}\frac{\partial\mathfrak{A}_\lambda(x)}{\partial x_\nu}+\frac{\partial\mathfrak{A}_\lambda(x)}{\partial x_\nu}\frac{\partial\mathfrak{A}_\lambda(x)}{\partial x_\mu}-\delta_{\mu\nu}\left(\frac{\partial\mathfrak{A}_\lambda(x)}{\partial x_\sigma}\right)^2\right]\\ &+\frac{\hbar}{2}\int_\sigma d\sigma_\mu\left[\bar\psi(x)\gamma_\mu\frac{\partial\psi(x)}{\partial x_\nu}-\frac{\partial\psi(x)}{\partial x_\nu}\bar\psi(x)\gamma_\mu\right],\end{aligned} \tag{2·12}$$

$$P_\nu^{(1)}[\sigma]=\frac{1}{c}\int_\sigma d\sigma_\nu\frac{1}{c}j_\mu(x)\mathfrak{A}_\mu(x), \tag{2·13}$$

and

$$P_\nu^{(2)}[\sigma]=\frac{1}{2c}\int_\sigma d\sigma_\nu d\sigma_\lambda' d\mathfrak{D}(x-x')\frac{1}{c}n_\mu j_\mu(x)\frac{1}{c}j_\lambda(x'). \tag{2·14}$$

The operator that describes the clothed photon is obtained by constructing the Heisenberg representation of $\mathfrak{A}_\mu(x)$,

$$\mathfrak{A}_\mu(x)=S^{-1}[\sigma]\,\mathfrak{A}_\mu(x)\,S[\sigma], \tag{2·15}$$

where $S[\sigma]$ is an unitary operator which transforms the field variables in the Heisenberg representation into those in the interaction representation. It is defined by the equation of motion

$$i\hbar c\frac{\delta S[\sigma]}{\delta\sigma(x)}=(H_1(x)+H_2(x))S[\sigma], \tag{2·16}$$

and the initial condition

$$S[-\infty]=1. \tag{2·17}$$

The explicit form was obtained by Dyson[7] as

$$S[\sigma]=1+(-i/\hbar c)\int_{-\infty}^{\sigma}(H_1(x)+H_2(x))dx+(-i/\hbar c)^2\int_{-\infty}^{\sigma}dx_1\int_{-\infty}^{\sigma(x_1)}(H_1(x_1)+H_2(x_1))$$
$$\times(H_1(x_2)+H_2(x_2))dx_2+\cdots\cdots. \tag{2·18}$$

$\mathfrak{A}_\mu(x)$ includes all effects of the interaction between the photon and the electron, and is the one that will describe the clothed photon correctly.

The equation of motion for $\mathfrak{A}_\mu(x)$ can be obtained from

$$\frac{\partial \boldsymbol{F}(x)}{\partial x_\nu}=S^{-1}[\sigma]\frac{\partial F(x)}{\partial x_\nu}S[\sigma]+(i/\hbar c)S^{-1}[\sigma]\int[H_1(x)+H_2(x),F(x')]d\sigma_\nu' S[\sigma].$$

With $F(x)=\partial\mathfrak{A}_\mu(x)/\partial x_\nu$, it is found that

$$\Box\mathfrak{A}_\mu(x)=(i/\hbar c)S^{-1}[\sigma]\int[H_1(x)+H_2(x),\partial\mathfrak{A}_\mu(x')/\partial x_\nu']d\sigma_\nu' S[\sigma]. \tag{2·19}$$

The integration of (2·19) yields

$$\Box\mathfrak{A}_\mu(x)=-\frac{1}{c}\left\{(\delta_{\mu\nu}+n_\mu n_\nu)\boldsymbol{j}_\nu(x)-\left(\frac{\partial}{\partial x_\mu}+n_\mu d\right)\varphi(x)\right\}, \tag{2·20}$$

where $\boldsymbol{j}_\mu(x)$ is the current vector operator in the Heisenberg representation

$$\boldsymbol{j}_\mu(x)=S^{-1}[\sigma]j_\mu(x)\,S[\sigma]=j_\mu(x)+(i/\hbar c^2)\int_{-\infty}^{\sigma}[j_\mu(x),j_\nu(x')]\mathfrak{A}_\nu(x')dx'+\cdots, \tag{2·21}$$

$\varphi(x)$ is defined by

$$\varphi(x)=\int_\sigma\left(\frac{\partial}{\partial x_\lambda'}+n_\lambda d'\right)\boldsymbol{j}_\lambda'\cdot\frac{\partial\mathfrak{D}(x-x')}{\partial x_\nu}d\sigma_\nu', \tag{2·22}$$

and we utilized an identity

$$\int_\sigma(\partial/\partial x_\mu+n_\mu d)(\partial/\partial x_\mu+n_\mu d)\frac{\partial\mathfrak{D}(x-x')}{\partial x_\nu}d\sigma_\nu'=1$$

in the course of the calculation. The right hand side of (2·20) represents the transverse part of the current vector $\boldsymbol{j}_\mu(x)$. Indeed we can show easily

$$n_\mu\{(\delta_{\mu\nu}+n_\mu n_\nu)\boldsymbol{j}_\nu(x)+(\partial/\partial x_\mu+n_\mu d)\varphi(x)\}=0\,,$$

and

$$\left(\frac{\partial}{\partial x_\mu}+n_\mu d\right)\left\{(\delta_{\mu\nu}+n_\mu n_\nu)\boldsymbol{j}_\nu(x)+(\partial/\partial x_\mu+n_\mu d)\varphi(x)\right\}=0\,.$$

The equation of motion for the field of the clothed photon in the free space is obtained by taking the expectation value of (2·20) in the vacuum state of the electron. Remembering that the vacuum expectation value of $j_\mu(x)$ vanishes, and anticipating the form (2·25) for $\delta j_\mu(x)$, the result is simplified to

$$\Box\langle\mathfrak{A}_\mu(x)\rangle_{\text{vac}}=-\frac{1}{c}\delta j_\mu(x) \tag{2·23}$$

in the e^2 approximation, where

$$\delta j_\mu(x)=\langle i/\hbar c^2\int_{-\infty}^{\sigma}[j_\mu(x),j_\nu(x')]\mathfrak{A}_\nu(x')dx'\rangle_{\text{vac}} \tag{2·24}$$

is the current induced in vacuum by the photon. It is a well known fact that, under the present stage of quantum electrodynamics, we can not avoid mathematical ambiguities in computing $\delta j_\mu(x)$. Hence we write the form

$$\frac{1}{c}\delta j_\mu(x)=2d^2\xi\left(\frac{1}{i}\frac{\partial}{\partial x_\mu}\right)\mathfrak{A}_\mu(x), \tag{2·25}$$

with the aid of an undetermined operator $\xi(1/i\cdot\partial/\partial x_\mu)$. The insertion of d^2 is merely to make $\xi(1/i\cdot i\partial/\partial x_\mu)$ dimensionless, and $\xi(1/i\cdot i\partial/\partial x_\mu)$ is a scalar quantity which shoulders the ambiguities due to the singular character of D functions. Different expressions have been given to $\xi(1/i\cdot i\partial/\partial x_\mu)$. It vanishes according to Schwinger's theory, but diverges quadratically in the usual perturbation calculation. We remark, however, that, whatever the form of $\xi(1/i\cdot i\partial/\partial x_\mu)$ may be, $\delta j_\mu(x)$ remains gauge invariant and satisfies the conservation law of charge on account of (2·5).

Expanding $\mathfrak{A}_\mu(x)$, $\mathfrak{A}_\mu(x)$ in Fourier series

$$\mathfrak{A}_\mu(x)=\sum\mathfrak{A}_\mu(k_\mu)e^{ik_\mu x_\mu}\,,$$

$$\mathfrak{A}_\mu(x)=\sum\mathfrak{A}_\mu(k_\mu)e^{ik_\mu x_\mu}\,, \tag{2·27}$$

let us consider hereafter a single component with a wave number k_μ. Substituting for $\delta j_\mu(x)$ the expression (2·25), (2·23) takes the following form for this component

$$\left(\sum_{j=1}^{3}k_j^2+k_4^2\right)\mathfrak{A}_\mu(k_\mu)=2(n_\mu k_\mu)^2\xi(k_\mu)\mathfrak{A}_\mu(k_\mu), \tag{2·28}*$$

which is written as

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* We replaced in the right hand side of (2·28) $\mathfrak{A}_\mu(k_\mu)$ by $\mathfrak{A}_\mu(k_\mu)$, since the difference is only of the order e^3 or higher.

$$\left(\sum_{j=1}^{3} k_j^2 + \frac{k_4^2}{(1-\xi(k_\mu))^2}\right)\mathfrak{A}_\mu(k_\mu) = 0\,. \tag{2·29}$$

The equation (2·29) shows that the velocity of a clothed photon with a wave number k_μ is altered to

$$c + \Delta c = (1-\xi(k_\mu))c\,, \tag{2·30}$$

as a result of the interaction.

§ 3. The energy and the momentum of a clothed photon

The energy and the momentum of the system can be calculated, including all effects of the interaction, by taking the expectation value of $P_\nu[\sigma]$;

$$\langle P_\nu[\sigma]\rangle = (\Psi[\sigma]^* P_\nu[\sigma]\Psi[\sigma]). \tag{3·1}$$

Assuming that the interaction is switched on adiabatically at $\sigma = -\infty$, we can write

$$\Psi[\sigma] = S[\sigma]\Psi[-\infty] \tag{3·2}$$

with $S[\sigma]$ given by (2·18). Inserting (3·2) into (3·1),

$$\langle P_\nu[\sigma]\rangle = (\Psi[-\infty]^* S^{-1}[\sigma] P_\nu[\sigma] S[\sigma]\Psi[-\infty]). \tag{3·3}$$

$\Psi[-\infty]$ being a free state by definition, the problem is reduced to the calculation of $S^{-1}[\sigma]\ P_\nu[\sigma]S[\sigma]$.

Employing an explicit form for $S[\sigma]$, the part of $S^{-1}[\sigma]P_\nu[\sigma]S[\sigma]$ that contributes to the energy and the momentum of a clothed photon is found as

$$\begin{aligned} S^{-1}[\sigma]P_\nu[\sigma]S[\sigma] = {} & P_\nu^{(0)}[\sigma] + (i/\hbar c)\int_{-\infty}^{\sigma} [H_1(x_1), P_\nu^{(0)}[\sigma]]\,dx_1 \\ & + (i/\hbar c)^2 \int_{-\infty}^{\sigma} dx_1 \int_{-\infty}^{\sigma(x_1)} [H_1(x_2), [H_1(x_1), P_\nu^{(0)}[\sigma]]]\,dx_2 \\ & + P_\nu^{(1)}[\sigma] + (i/\hbar c)\int_{-\infty}^{\sigma} [H_1(x_1), P_\nu^{(1)}[\sigma]]\,dx_1 \end{aligned} \tag{3·4}$$

in the e^2 approximation as before.

The calculation of (3·4) can be facilitated by utilizing the fact that $P_\nu^{(0)}[\sigma]$ is a translation operator for $\psi(x)$ and $\mathfrak{A}_\mu(x)$:

$$i/\hbar[\psi(x), P_\nu^{(0)}[\sigma]] = \partial\psi(x)/\partial x_\nu\,, \tag{3·5}$$

$$i/\hbar[\mathfrak{A}_\xi(x), P_\nu^{(0)}[\sigma]] = \partial\mathfrak{A}_\xi(x)/\partial x_\nu\,. \tag{3·6}$$

The proof of (3·5) is given in Schwinger's paper. We can also verify (3·6) in an analogous way.

We first observe

$$\begin{aligned} & i/\hbar\int_\sigma [\mathfrak{A}_\xi(x), \partial\mathfrak{A}_\lambda(x')/\partial x_\mu' \cdot \partial\mathfrak{A}_\lambda(x')/\partial x_\nu']\,d\sigma_\mu' \\ & \quad = -c\int_\sigma\Big[\Big\{\delta_{\xi\lambda}\frac{\partial D(x-x')}{\partial x_\mu'} + n_\xi n_\lambda \frac{\partial D(x-x')}{\partial x_\mu'} \end{aligned}$$

$$-(\partial/\partial x_\xi'+n_\xi d')(\partial/\partial x_\lambda'+n_\lambda d')\frac{d'\mathfrak{D}(x-x')}{\partial x_\mu'}\Big\}\frac{\partial\mathfrak{A}_\lambda(x')}{\partial x_\nu'}$$

$$+\Big\{\delta_{\xi\lambda}\frac{\partial D(x-x')}{\partial x_\nu'}+n_\xi n_\lambda\frac{\partial D(x-x')}{\partial x_\nu'}$$

$$-(\partial/\partial x_\xi'+n_\xi d')(\partial/\partial x_\lambda'+n_\lambda d')\frac{\partial\mathfrak{D}(x-x')}{\partial x_\nu'}\Big\}\frac{\partial\mathfrak{A}_\lambda'(x')}{\partial x_\mu'}\Big]d\sigma_\mu'.$$

The second terms in each bracket vanish by virtue of (2·5), and the third terms are also shown to vanish by the same reason after an integration by parts, which is permitted since $(\partial/\partial x_\mu'+n_\mu d')$ is a spatial differentiation and $d\sigma_\nu'$ is a spatial integration. Hence

$$i/\hbar\int\Big[\mathfrak{A}_\xi(x),\frac{\partial\mathfrak{A}_\lambda(x')}{\partial x_\mu'}\frac{\partial\mathfrak{A}_\lambda(x')}{\partial x_\nu'}\Big]d\sigma_\mu'$$

$$=c\int_\sigma\Big(\frac{\partial D(x-x')}{\partial x_\mu}\frac{\partial\mathfrak{A}_\xi(x')}{\partial x_\nu'}+\frac{\partial D(x-x')}{\partial x_\nu}\frac{\partial\mathfrak{A}_\xi(x')}{\partial x_\mu'}\Big)d\sigma_\mu',$$

and

$$i/\hbar[\mathfrak{A}_\xi(x),P_\nu^{(0)}[\sigma]]=\int_\sigma\Big\{\frac{\partial D(x-x')}{\partial x_\mu}\frac{\partial\mathfrak{A}_\xi(x')}{\partial x_\nu'}+\frac{\partial D(x-x')}{\partial x_\nu}\frac{\partial\mathfrak{A}_\xi(x')}{\partial x_\mu'}$$

$$-\delta_{\mu\nu}\frac{\partial D(x-x')}{\partial x_\sigma}\frac{\partial\mathfrak{A}_\xi(x')}{\partial x_\sigma'}\Big\}d\sigma_\mu',$$

which can be written as

$$i/\hbar[\mathfrak{A}_\xi(x),P_\nu^{(0)}[\sigma]]=\int_\sigma\Big\{\frac{\partial D(x-x')}{\partial x_\mu}\frac{\partial\mathfrak{A}_\xi(x')}{\partial x_\nu'}-D(x-x')\frac{\partial^2\mathfrak{A}_\xi(x)}{\partial x_\mu'\partial x_\nu'}\Big\}d\sigma_\mu'.$$

It is easy to show that this expression is independent of σ, and we find, by choosing as σ a space like surface through x, that

$$i/\hbar[\mathfrak{A}_\xi(x),P_\nu^{(0)}[\sigma]]=\partial\mathfrak{A}_\xi(x)/\partial x_\nu.$$

It is a direct result of (3·5) and (3·6) that we can write

$$i\int_{-\infty}^{\sigma}[H_1(x_1),P_\nu^{(0)}[\sigma]]dx_1=\int_\sigma H_1(x)d\sigma_\nu. \tag{3·7}$$

For the calculation of the next term of (3·4), it is convenient first to rearrange the factors in the form;

$$(i/\hbar c)^2\int_{-\infty}^{\sigma}dx_1\int_{-\infty}^{\sigma(x_1)}dx_2[H_1(x_2),[H_1(x_1),P_\nu^{(0)}[\sigma]]]$$

$$=\frac{1}{2}(i/\hbar c)^2\int_{-\infty}^{\sigma}dx_1\int_{-\infty}^{\sigma(x_1)}\{[H_1(x_2)H_1(x_1),P_\nu^{(0)}[\sigma]]-[H_1(x_1)H_1(x_2),P_\nu^{(0)}[\sigma]]\}dx_2$$

$$+\frac{1}{2}(i/\hbar c)^2\iint_{-\infty}^{\sigma}[H_1(x_2),[H_1(x_1),P_\nu^{(0)}[\sigma]]]dx_1dx_2.$$

The first integral does not contribute to the result, since $\Psi[-\infty]$ is an eigenstate of $P_\nu^{(0)}[\sigma]$, and the second is transformed into

$$\frac{1}{2}(i/\hbar c)\int_\sigma d\sigma_\mu \int_{-\infty}^{\sigma}[H_1(x_1), H_1(x)]dx_1$$

on account of (3·5) and (3·6). We thus find as the contributions to $S^{-1}[\sigma]P_\nu[\sigma]S[\sigma]$ from $P_\nu^{(0)}[\sigma]$

$$P_\nu^{(0)}[\sigma]+\int_\sigma H_1(x)d\sigma_\nu+\frac{i}{2}(i/\hbar c)\int_\sigma d\sigma_\nu\int_{-\infty}^{\sigma}[H_1(x_1), H_1(x)]dx_1 . \quad (3\cdot 8)$$

The evaluation of the contributions from $P_\nu^{(1)}[\sigma]$ is very simple, and the result is

$$-\int_\sigma H_1(x)d\sigma_\mu-(i/\hbar c)\int_\sigma d\sigma_\mu\int_{-\infty}^{\sigma}[H_1(x_1), H_1(x)]dx_1 . \quad (3\cdot 9)$$

Adding (3·8) and (3·9)

$$S^{-1}[\sigma]P_\nu[\sigma]S[\sigma]=P_\nu^{(0)}[\sigma]-\frac{1}{2}(i/\hbar c)\int_\sigma d\sigma_\mu\int_{-\infty}^{\sigma}[H_1(x_1), H(x)]dx_1 . \quad (3\cdot 10)$$

Picking up from (3·10) those terms only which contribute to the energy and the momentum of a clothed photon,

$$S^{-1}[\sigma]P_\nu[\sigma]S[\sigma]=P_\nu^{(0)}[\sigma]-\frac{1}{4c}\int_\sigma\{\delta j_\mu(x)\mathfrak{A}_\mu(x)+\mathfrak{A}_\mu(x)\delta j_\mu(x)\}d\sigma_\nu , \quad (3\cdot 11)$$

using $\delta j_\mu(x)$ given by (2·24).

Thus, taking a flat surface for σ, the energy and the momentum of a clothed photon are obtained to be

$$E+\Delta E=(\Psi^*[-\infty]\,(-iP_4[\sigma]+\frac{1}{4c}\int_\sigma\{\delta j_\mu(x)\mathfrak{A}_\mu(x)+\mathfrak{A}_\mu(x)\delta j_\mu(x)\}dv)\,\Psi[-\infty]),$$
$$p_j+\Delta p_j=(\Psi^*[-\infty]\,P_j\,\Psi[-\infty]), \quad (3\cdot 12)$$
$$(j=1, 2, 3).$$

With $\delta j_\mu(x)$ assumed in the form (2·25), and n_μ chosen as $(0, 0, 0, i)$, we finally find that the energy and the momentum of a clothed photon with a wave number k_μ are given by

$$E+\Delta E=(1-\xi(k_\mu))E ,$$
and
$$p+\Delta p=p . \quad (3\cdot 13)$$

§ 4. Renormalization of the light velocity

Collecting the results (3·13) and (2·30), and remembering that Einstein's relation $E=pc$ holds for the free parts, we find that

$$E+\Delta E=p(c+\Delta c) \quad (4\cdot 1)$$

is satisfied between $E+\Delta E$, p, and $c+\Delta c$. This is just what was anticipated in the introduction. It should also be noted that this identity is not suffered from the mathematical ambiguities which were encountered in the calculation of $\delta j_\mu(x)$. We shall develop a concrete

renormalization procedure of the light velocity in this section on the ground of this identity.

The Hamiltonian of the electromagnetic field is given by

$$H=-iP_4=\frac{1}{2}\int(\boldsymbol{E}^2+\boldsymbol{H}^2)dv=\frac{1}{2}\int\left\{(\mathrm{curl}\,\mathfrak{A})^2+\frac{1}{c^2}\left(\frac{\partial\mathfrak{A}}{\partial t}\right)^2\right\}dv'. \qquad (4\cdot2)^*$$

Regarding $(4\cdot2)$ as a function of c, we can rewrite it in the form;

$$H(c)=H(c+\Delta c)-\frac{\partial H}{\partial c}\Delta c.$$

The indicated calculation can be performed unambiguously if we restrict our attention to a single Fourier component of $\mathfrak{A}_\mu(x)$ with a wave number k_μ. Inserting for Δc the value given by $(2\cdot26)$,

$$H=\frac{1}{2}\int\left\{(\mathrm{curl}\,\mathfrak{A})^2+\frac{1}{(c+\Delta c)^2}\left(\frac{\partial\mathfrak{A}}{\partial t}\right)^2-\frac{2}{c^2}\left(\frac{\partial\mathfrak{A}}{\partial t}\right)\tilde{\xi}\left(\frac{1}{i}\frac{\partial}{\partial x_\mu}\right)\cdot\left(\frac{\partial\mathfrak{A}}{\partial t}\right)\right\}dv'.$$

We replace $c+\Delta c$ by c_{ob}, and treat

$$H(c_{ob})=\frac{1}{2}\int\left\{(\mathrm{curl}\,\mathfrak{A})^2+\frac{1}{c_{ob}^2}\left(\frac{\partial\mathfrak{A}}{\partial t}\right)^2\right\}dv, \qquad (4\cdot3)$$

as a Hamiltonian of the free clothed photon, while

$$-\frac{1}{c^2}\int\left(\frac{\partial\mathfrak{A}}{\partial t}\right)\tilde{\xi}\left(\frac{1}{i}\frac{\partial}{\partial x_\mu}\right)\left(\frac{\partial\mathfrak{A}}{\partial t}\right)^2dv \qquad (4\cdot4)$$

is regarded as a new counter term to cancel divergent effects produced by $j_\mu(x)\,\mathfrak{A}_\mu(x)$ interaction. Some remarks are necessary in removing the restriction imposed on the above derivation of $(4\cdot4)$. As repeated in previous sections, $\tilde{\xi}(k_\mu)$ is an ambiguous quantity and we do not know whether it is independent of k_μ or not. If it depends on k_μ, it would be difficult to perform the above renormalization procedure consistently for all wave numbers, since neither c nor c_{ob} is likely to depend on k_μ. To avoid this difficulty, it is necessary to give up to relate the counter term $(4\cdot4)$ with Δc in the Hamiltonian of the free clothed photon. That is, in generating the interaction adiabatically, we consider that c is altered to $c+\Delta c$, and at the same time we add, logically independent of the alteration of c, a new interaction term $(4\cdot4)$ to the ordinary interactions. Although if $\tilde{\xi}(k_\mu)$ is independent of k_μ, the effect of the alteration of c is just canceled by the new interaction and no new interaction is introduced, this cancellation can not be assured under the present stage of quantum electrodynamics. Thus our renormalization procedure differs from that of Tomonaga or Schwinger in that it results in the possible introduction of a new interaction. With these remarks in mind, let us consider $(4\cdot4)$ as a counter term in our theory. This can be written at once in an invariant form

$$-\frac{1}{c^2}d\mathfrak{A}_\mu(x)\cdot\tilde{\xi}\left(\frac{1}{i}\frac{\partial}{\partial x_\mu}\right)\cdot d\mathfrak{A}_\mu(x), \qquad (4\cdot5)$$

* $\mathfrak{A}$ used in this section without vector suffix means the space component of $\mathfrak{A}_\mu(x)$.

and in our theory the interacting system of the electromagnetic and electron fields is described by the Schrödinger equation

$$i\hbar c\frac{\delta\Psi[\sigma]}{\delta\sigma(x)}=\left\{-\frac{1}{c}j_\mu(x)\mathfrak{A}_\mu(x)-\frac{1}{2}\int\left\{\frac{1}{2}\frac{\partial}{\partial x_\mu}+n_\mu d'\right\}\mathfrak{D}(x-x')\frac{1}{c}j_\mu(x)\frac{1}{c}\right.$$
$$\left.\times j_\lambda(x')d\sigma_\lambda'-\frac{1}{c^2}d'\mathfrak{A}_\mu(x)\cdot\xi\left(\frac{1}{i}\frac{\partial}{\partial x_\mu}\right)\cdot d'\mathfrak{A}_\mu(x)^2\right\}\Psi[\sigma],\qquad(4\cdot6)^*$$

where $\mathfrak{A}_\mu(x)$ and $\psi(x)$ are the field variables which satisfy the equations of motion and the commutation relations of the form of $(2\cdot2)$ and $(2\cdot3)$ in which c is replaced by the observed value.

Disregarding a meaningless four dimensional divergence term, the new counter term $(4\cdot5)$ can be written as

$$\frac{1}{2c^2}\left\{d'^2\xi\left(\frac{1}{i}\frac{\partial}{\partial x_\mu}\right)\mathfrak{A}_\mu(x)\cdot\mathfrak{A}_\mu(x)+\mathfrak{A}_\mu(x)\cdot d'^2\xi\left(\frac{1}{i}\frac{\partial}{\partial x_\mu}\right)\mathfrak{A}_\mu(x)\right\},$$

which is further transformed, remembering the definition of $\delta j_\mu(x)$ $(2\cdot25)$, into

$$\frac{1}{4c}\{\delta j_\mu(x)\mathfrak{A}_\mu(x)+\mathfrak{A}_\mu(x)\delta j_\mu(x)\}.$$

This is nothing but the minus of the one photon part of the second order contribution to the interaction Hamiltonian caused by $j_\mu(x)\mathfrak{A}_\mu(x)$ interaction. Therefore the effects of the induced current, to the one photon part of the interaction Hamiltonian which were the origins of various difficulties vanish entirely in our theory.

§ 5. Lagrangian formalism of the theory

In view of the analysis of the preceding sections, we assume that the Lagrangian of the interacting system of the electromagnetic and electron fields is given by

$$L=L_0+\frac{1}{c}j_\mu(x)A_\mu(x)+\frac{1}{c^2}d'\mathfrak{A}_\mu(x)\cdot\xi\left(\frac{1}{i}\frac{\partial}{\partial x_\mu}\right)\cdot d'\mathfrak{A}_\mu(x)+\delta\varkappa\bar{\psi}(x)\psi(x),\quad(5\cdot1)$$

where

$$L_0=-\frac{1}{2}\frac{\partial A_\mu(x)}{\partial x_\nu}\frac{\partial A_\mu(x)}{\partial x_\nu}-\frac{1}{2}\bar{\psi}(x)\left(\gamma_\mu\frac{\partial}{\partial x_\mu}+\varkappa\right)\psi(x)-\frac{1}{2}\bar{\psi}'(x)\left(\gamma_\mu\frac{\partial}{\partial x_\mu}+\varkappa\right)\psi'(x)\qquad(5\cdot2)$$

is the Lagrangian of the free fields, c and $\varkappa$ the observed values of the light velocity and the electron mass respectively, and we appended with $\frac{1}{c^2}d'\mathfrak{A}_\mu(x)\cdot\xi\left(\frac{1}{i}\frac{\partial}{\partial x_\mu}\right)d'\mathfrak{A}_\mu(x)$ a mass counter term $\delta\varkappa\bar{\psi}(x)\psi(x)$.

Owing to the complicated nature of $\xi(1/i\cdot\partial/\partial x_\mu)$, it is difficult to write down the canonical formalism. We therefore perform the quantization following a generalized procedure proposed by Kanesawa and Koba. According to them, the Schrödinger equation of the system is assumed to be

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* Strictly speaking, normal dependent terms are necessary on the right hand side of $(4\cdot6)$ to secure the integrability. But it is easily shown that such terms are of the order c^3 or higher, and are neglected for the time being. Detailed discussion will be given in § 5.

$$i\hbar c\frac{\delta\Psi[\sigma]}{\delta\sigma(x)}=-L[x,\sigma]\Psi[\sigma], \tag{5·3}$$

where $L[x,\sigma]$ is determined directly from the interaction Lagrangian density $L(x)$ so that it satisfies

$$\frac{\delta L[x,\sigma]}{\delta\sigma(x')}-\frac{\delta L[x',\sigma]}{\delta\sigma(x)}=-\frac{i}{\hbar c}[L[x,\sigma],\ L[x',\sigma]] \tag{5·4}$$

when x and x' are space like to each other. Variables contained in $L[x,\sigma]$ are the solutions of the free field equations and satisfy the same commutation relations as the free ones. The solution of (5·4) was found in a power series of e

$$L[x,\sigma]=\sum_{m=1}^{\infty}e^m\{\sum_{n=1}^{m}L^{(n)(m-n)}[x,\sigma]\}. \tag{5·5}$$

corresponding to the interaction Lagrangian density which was assumed in the form;

$$L(x)=\sum_{j=1}^{m}e^{j+1}L^{(1)(j)}(x). \tag{5·6}$$

In (5·5) $L^{(n)(m-n)}[x,\sigma](n=1,\ m=1,\ 2,\cdots m)$ are equal to $L^{(1)(j)}(x)(j=1,\ 2,\cdots m)$ of (5·6), and other coefficient $L^{(n)(m-n)}[x,\sigma](n\geqq 2$, or $n=1,\ m=m+1,\cdots)$ are determined successively term by term from $L^{(n)(m-n)}[x,\sigma](n=1,\ m=1,\ 2,\cdots m)$. It is verified first that

$$\begin{aligned}
&\sum_{r=1}^{n-1}\sum_{k=0}^{m-n}[L^{(r)(k)}[x,\sigma],\ L^{(n-r)(m-n-k)}[x',\sigma]]\\
&=\sum_{J=\mathrm{I,II}}\Big[\{{}_JF^{(2)(n)(m-n)}_{\lambda\mu}[x,N]+{}_JF^{(2)(n)(m-n)}_{\lambda\mu\nu}[x,N](x_\nu-x_\nu')+\cdots\}\frac{\partial^2D(x-x')}{\partial x_\mu'\partial x_\nu'}\\
&+\{{}_JF^{(3)(n)(m-n)}_{\lambda\mu\nu}[x,N]+{}_JF^{(3)(n)(m-n)}_{\lambda\mu\nu\sigma}[x,N](x_\sigma-x_\sigma')+\cdots\}\frac{\partial^3D(x-x')}{\partial x_\nu'\partial x_\mu'\partial x_\lambda'}+\cdots\Big]\\
&-\sum_{J=\mathrm{I,II}}[x'\ x]
\end{aligned} \tag{5·7}*$$

where $F_{\lambda\mu}[x,N]$, $F_{\lambda\mu\nu}[x,N]\cdots$ mean respectively the second, the third$\cdots$ rank tensors composed of the field variables and their derivatives at the point x. The notation $\sum_{J=\mathrm{I\,II}}[x,x']$ on the right hand side is used for the expression obtained by changing x and x' in the first term of the same equation. The explicit form of (5·5) is written down with these $F_{\lambda\mu}[x,N]$, $F_{\lambda\mu\nu}[x,N]$,$\cdots\cdots$ as

$$\begin{aligned}
L[x,\sigma]&=L(x)-\frac{i}{\hbar c}\sum_{n=2}e^m[\sum_{m=2}^{m}\sum_{J=1}^{\mathrm{II}}\\
&\times\Big[(N_\lambda N_\mu\,{}_JF^{(2)(n)(m-n)}_{\lambda\mu}[x,N]+\Big(N_\nu\frac{\partial N_\lambda}{\partial x_\mu}+N_\mu\frac{\partial N_\lambda}{\partial x_\nu}\Big)\,{}_JF^{(3)(n)(m-n)}_{\lambda\mu\nu}[x,N]\\
&+(N_\mu N_\nu\delta_{\lambda\sigma}+N_\nu N_\lambda\delta_{\mu\sigma}+N_\lambda N_\mu\delta_{\nu\sigma})\,{}_JF^{(n)(m-n)}_{\lambda\mu\nu\sigma}[x,N]+\cdots\cdots\Big].
\end{aligned} \tag{5·8}$$

Starting from $L(x)$, and using (5·7) and (5·8) repeatedly, all terms of the series (5·5) can be calculated to any desired order.

Application of the above discussion to our system can be done at once where the interaction Lagrangian density is given by

* N_μ means the normal vector of the space like surface σ.

$$L(x)=\frac{1}{c}j_\mu(x)A_\mu(x)+\frac{1}{c^2}d\mathfrak{A}_\mu(x)\cdot\xi\left(\frac{1}{i}\frac{\partial}{\partial x_\mu}\right)d\mathfrak{A}_\lambda(x)^2+\delta x\bar{\psi}(x)\psi(x). \tag{5·9}$$

The field variable satisfies the following equations of motion and the commutation relations

$$\Box A_\mu(x)=0,$$

$$\left(\gamma_\mu\frac{\partial}{\partial x_\mu}+\varkappa\right)\Psi=0, \tag{5·10}$$

$$[A_\mu(x),\ A_\nu(x')]=i\hbar c\delta_{\mu\nu}D(x-x'),$$

$$[\psi_\alpha(x),\ \bar{\psi}_\beta(x')]=\frac{1}{i}S_{\alpha\beta}(x-x'), \tag{5·11}$$

in which we must use observed values for c and $\varkappa$.

It is convenient to perform a canonical transformation

$$\Psi[\sigma]\to U[\sigma]\Psi[\sigma],$$

$$U[\sigma]=e^{i/\hbar c\int_\sigma j_\mu(x)A'(x)d\sigma_\mu} \tag{5·12}$$

beforehand. After the transformation, $L(x)$ is transformed into

$$\bar{L}(x)=U[\sigma]L(x)U^{-1}[\sigma]-i\hbar cU[\sigma]\frac{\delta U^{-1}[\sigma]}{\delta\sigma(x)}$$

$$=\frac{1}{c}j_\mu(x)\mathfrak{A}_\mu(x)+\frac{1}{2}\int_\sigma\left(\frac{1}{2}\frac{\partial}{\partial x_\mu}+n_\mu d\right)\mathfrak{D}(x-x')\frac{1}{c}j_\mu(x)\frac{1}{c}j_\lambda(x')d\sigma_\lambda'$$

$$+\frac{1}{c}n_\mu j_\mu(x)d(A(x)-A'(x))+\frac{1}{c^2}d\mathfrak{A}_\mu(x)\cdot\xi\left(\frac{1}{i}\frac{\partial}{\partial x_\mu}\right)\cdot d\mathfrak{A}_\mu(x)+\delta x\bar{\psi}(x)\psi(x). \tag{5·13}$$

It should be noted that in the transformed interaction Lagrangian density $A(x)$ and $A'(x)$ appear only in a combined form $(A(x)-A'(x))$. A characteristic feature of this combination is express by

$$[A(x)-A'(x),\ A(x')-A'(x')]=0, \tag{5·14}$$

which is a direct result of the commutation relation (5·11). Thus, in constructing $F_{\lambda\mu}[x,N]$, $F_{\lambda\mu\nu}[x,N]$,..... from (5·13) according to (5·7), no term appear which contain $A(x)$ or $A'(x)$.

Therefore we can write $L[x,\sigma]$ in the form

$$L[x,\sigma]=\frac{1}{c}j_\mu(x)\mathfrak{A}_\mu(x)+\int\left(\frac{1}{2}\frac{\partial}{\partial x_\mu}+n_\mu d\right)\mathfrak{D}(x-x')\frac{1}{c}j_\mu(x)\frac{1}{c}j_\lambda(x')d\sigma_\lambda'$$

$$+n_\mu j_\mu(x)d(A(x)-A'(x))+\frac{1}{c^2}d\mathfrak{A}_\mu(x)\cdot\xi\left(\frac{1}{i}\frac{\partial}{\partial x_\mu}\right)\cdot d\mathfrak{A}_\mu(x)$$

$$+\delta x\bar{\psi}(x)\psi(x)+W[x,\sigma], \tag{5·15}$$

$$W[x,\sigma]=\sum_{m=3}^{\infty}e^m w^{(m)}[x,\sigma], \tag{5·16}*$$

with $W^{(n)}[x,\sigma]$ which does not contain $A(x)$ or $A'(x)$.

* $W^{(2)}[x,\sigma]$ vanishes in (5·16). The reason is the commutability of $j_\mu(x)\mathfrak{A}_\mu(x)$ with $j_\mu(x')\mathfrak{A}_\mu(x')$ for x and x' which are space like to each other.

We further impose a subsidiary condition on $\Psi[\sigma]$;

$$(\Lambda(x)-\Lambda'(x))\Psi[\sigma]=0\,. \tag{5·17}$$

The compatibility of (5·17) with the Schrödinger equation is obvious from (5·14) and from the fact that $w^{(m)}[x,\sigma]$ does not contains $\Lambda(x)$ or $\Lambda'(x)$. With the solution of $L[x,\sigma]$ obtained in the form of (5·15), and under the subsidiary condition (5·17), we finally find that the Schrödinger equation of our system is given by

$$i\hbar c\frac{\delta\Psi[\sigma]}{\delta\sigma(x)}=\Big\{-\frac{1}{c}j_\mu(x)\mathfrak{A}_\mu(x)-\int\Big(\frac{1}{2}\frac{\partial}{\partial x_\mu}+n_\mu d\Big)$$

$$\times\mathfrak{D}(x-x')\frac{1}{c}j_\mu(x)\frac{1}{c}j_\lambda(x')d\sigma'_\lambda$$

$$-\frac{1}{c^2}d\mathfrak{A}_\mu(x)\cdot\xi\Big(\frac{1}{i}\frac{\partial}{\partial x_\mu}\Big)\cdot d\mathfrak{A}_\mu(x)-\delta\varkappa\bar{\psi}(x)\psi(x)-W[x,\sigma]\Big\}\Psi[\sigma]\,. \tag{5·18}$$

In our theory the interacting system of the electromagnetic and electron fields is described by the Schrödinger equation (5·18) and the supplementary condition (5·17) constructed from field variables which satisfy the equations of motion (5·10) and the commutation relations (5·1). The result of this sections coincides with those of the preceding sections in the e^2 approximation. We thus arrive at a complete description of the interaction of the electro-magnetic and electron fields which is manifestly Lorentz- and gauge invariant, and is free from the divergence of the self-energy of the photon or the electron.

§ 6. Concluding remarks

Thus far we have shown a possibility of dissolving the self-energy difficulty of the photon by the idea of renormalizing the light velocity. Our attempt may seem strange at first sight. Lorentz transformation, however, was a result of recognizing that it is a nonsense to conceive of the structure of the space-time without reference to the actual measure to define it. Thus it seems to us a very natural course to use, if we admit Einstein's philosophy, the observed value of c which includes the effect of interaction, as a natural constant to characterize Lorents transformation, although objections may be raised against this positivistic standpoint.

In § 4 we remarked that our renormalization procedure might result in the introduction of a new interaction. It is quite a open problem whether such a drastic modification of the current theory is really necessary, and even if our attempt is on the right way in its essential part, we would have to resort to future theories to manage the divergence of Δc. With all such unsatisfactory features of our theory, however, we want to emphasize that the self-energy problem of the photon would not be settled by computing the self-energy alone, for, whether the rest mass of the photon vanishes or not is a question decided by whether Einstein's relation $E=pc$ is satisfied between E, p and c or not, not by whether the self-energy vanishes or not. Thus it would be necessary for the ultimate solution of the problem to consider the effect of the interaction upon the momentum and the velocity of the photon in addition to the computation of the self-energy, and, in

particular, it seems inadmissible to ignore the alteration of the velocity so long as the self-energy terms survive, for, as will be seen from the calculation of § 2 and § 3, they are both the result of the induced current and are inevitably related to each other.

In this paper we discussed only the interaction of the electromagnetic field with the electron field, but the situation is essentially the same even if we take into account any kind of charged field provided that the interaction is introduced in a gauge invariant way. In such a case Δc becomes a sum of contributions from all charged fields which interact with the electromagnetic field. Further, considering the effects of higher order, even neutral fields give contribution to Δc. For example, contributions from neutral meson field would appear in the e^2g^2 approximation from its interaction with nucleons in the intermediate state. We must, therefore, conclude that behind the observed value of c the mechanism of all interactions of all elementary particles that exist in the nature lie hidden, and the contributions from them are all condensed into this value of c.

We finally give a brief discussion on those fields of vanishing machanical rest mass other than the electromagnetic field. If there is no interaction, any field that has a vanishing rest mass could be used as a signal in Einstein's theory. When interactions are introduced, their propagation velocity will be altered, and, if the alterations are not the same for all such fields, there would be a paradoxical situation, since it would imply the existence of different values of c to be taken into Lorentz transformation. The situation is not so troublesome, however, for if we do not consider fields with spin higher than 3/2, electromagnetic field is the only one that possesses invariance under a gauge transformation. Thus, for example, although the mechanical mass of the neutrino is presumably zero, its self-energy can be interpreted as the rest mass, and, when we take into account the effect of the interaction, neutrino loses its qualification as a signal in Einstein's theory. The photon has a peculiar character in that it has exactly a vanishing rest mass even when it interacts with other fields, and is the only one that can be used as a signal.

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References

1) J. Schwinger, Phys. Rev. **74** (1948), 1439.
J. Schwinger, Phys. Rev. **75** (1949), 651.
2) W. Pauli and F. Villars, Rev. Mod. Phys. **21** (1949), 434.
3) H. Umezawa, J. Yukawa and E. Yamada, Prog. Theor. Phys. **4** (1949), 25.
4) D. Feldman, Phys. Rev. **76** (1949), 1367.
5) S. Tomonaga and T. Tati, Prog. Theor. Phys. **3** (1948), 391.
6) F. J. Dyson, Phys. Rev. **75** (1949), 486.
7) S. Kanesawa and Z. Koba, Prog. Theor. Phys. **4** (1949), 297.

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The Theory of the Dielectric Constant of Ionic Crystals, I

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We worked out the dielectric constants of $\varkappa_0$ and $\varkappa$ of the alkali-halide crystal on the basis of the quantum theory of solids. We have used the variational method of Slater and Kirkwood in our energy-calculations and adopted Landshoff's method for evaluating the exchange integrals among the non-orthogonal wave functions. The relation among the various theories, due to Shockley, Mott and Fröhlich, of the dielectric constant of ionic crystal have been clarified from the viewpoint of our theory. The numerical results for LiF are in good accordance with the experiment.

§ 1. Introduction[1)]

Many of the characteristic properties of polar crystals, i.e., the behaviour of the conduction electrons or the existence of defects in the lattice will, after all, sensitively depend on the dielectric properties of the crystal. So we see it is essentially required to elucidate the dielectric properties of the mentioned crystals in detail on the basis of the quantum theory of solids, since the available theories of dielectric properties are usually based on the rather phenomenological considerations. As a preliminary to the general formulation of the theory we shall here work quantum-mechanically the simplest case of the dielectric constant of ionic crystals in the homogeneous external fields of both high frequency and static natures.

As is well-known in the classical theory, the relation between the polarizability (α) of an ion pair and the dielectric constant ($\varkappa_0$) for high frequency field is represented by one or the other of the following two formulae according to the assumptions of the effective field $\boldsymbol{F}_{eff}$ around each ion of the crystal. Namely, we have

$$\varkappa_0-1=4\pi N\alpha \qquad \text{(the Drude formula)} \quad \cdots\cdots\cdots \quad (1)$$

and

$$\varkappa_0-1/\varkappa_0+2=4\pi N\alpha/3, \qquad \text{(the Lorentz-Lorenz formula)} \quad (2)$$

where N is the number of ion pairs per unit volume. These formulae are well-recognized to depend on the field that is assumed to be effective in polarizing each ion. Let us denote by $\boldsymbol{P}$ the polarization of the medium and by $\boldsymbol{F}$ the external electric field, then one of the assumptions,

$$F_{eff}=F, \qquad (3)$$

leads to the Drude formula (1), and the other one

$$F_{eff}=F+\frac{4\pi}{3}P, \tag{4}$$

to the Lorentz-Lorenz formula (2).

The justification of the assumption (4) has been given by Lorentz and Fowler, using the simplified model of point-dipole lattice, in which the field at any one lattice point due to all the other dipoles within the crystal may be evaluated. As far as the above mentioned model of crystal is used, the Lorentz-Lorenz formula is shown to be valid for the lattice of any cubic structure.

Recently, Mott has developed the theory of the dielectric constant on the basis of Born's lattice dynamics together with the detailed discussions of the observed values of alkali-halides. According to him the Drude formula has been shown to give a better agreement with the observation compared with the Lorentz-Lorenz formula. Furthermore, he pointed out that the assumption of the point dipole is by no means guaranteed for the contribution of the nearest neighbouring ions to the effective field, because the ion clouds are somewhat overlapping with each other in the actual cases. Taking account of these circumstances, Mott proposed that the effective field is given by the modified formula

$$F_{eff}=F+\frac{4\pi}{3}\gamma P, \tag{5}$$

where γ is the numerical factor less than unity. As one is not able to derive the value of γ within the frame of the Mott's theory, the value of γ has to be determined to obtain a best fitting with the observed value of dielectric constant, according to which γ has been shown to become almost zero in alkali-halides.

According to Shockley, on the other hand the Lorentz formula may still provide correctly the observed value of $\varkappa_0$ for many ionic crystals, if the polarizability of each ion is given a suitable value. In view of the unsettled situations regarding the effective field within the crystal, we shall attempt here to work the problem in question on the sound basis of the quantum theory of solids.

§ 2 The method of computation

Now we show our method of computation of the dielectric constants for the cases of LiF and MgO. We may be allowed to assume tentatively that these substances are almost purely ionic crystals in working the dielectric properties. As is well-known, we have the relation between the dielectric constant $\varkappa$ (or $\varkappa_0$) and the energy change ΔE under the influence of a homogeneous external field F

$$\Delta E=-\frac{1}{2}\chi F^2 \tag{6}$$

and

$$\varkappa-1=4\pi N\chi\,. \tag{7}$$

In order to compute the energy change ΔE, we have now two methods of treatment, one is the usual 2nd order perturbation method and the other the variational one, the latter of which has been used by Hasse[2] or Slater and Kirkwood[3] for calculating the polarizability of He atom. We shall here make use of the method of Slater and Kirkwood to calculate the total energy of the crystal with the external field. Now the total energy of the crystal without the application of an external field consists of three parts:

$$E=E_0+E_1+E_2, \tag{8}$$

where E_0 is the energy of the positive and negative ions in free state, E_1 the electrostatic mutual interaction energy among them and E_2 the exchange energy between the ions. In the previous papers[4,5] we have actually calculated the total crystal energies for both LiF and MgO, and then determined the available forms of wave functions of negative ions by the variational method. When the external electric field F is existing, the total crystal energy changes by ΔE, which also consists of three parts corresponding to eq. (8)

$$\Delta E=\Delta E_0+\Delta E_1+\Delta E_2, \tag{9}$$

where ΔE_0 is the energy change of the positive and negative ions in free state, ΔE_1 the change of the electrostatic interaction energy and ΔE_2 the change of the exchange energy respectively under the influence of the external field. According to Slater and Kirkwood we shall assume the wave function for $2p$-electron of F^- ion as follows[4]:

$$\begin{aligned}\psi&=\psi_0(\boldsymbol{r})\,(1+\lambda r\cos\theta)\\&=(P(r)/r)\,(1+\lambda r\cos\theta)\begin{Bmatrix}\cos\theta\\ \sin\theta\ \cos\phi\\ \sin\theta\ \sin\phi\end{Bmatrix},\end{aligned} \tag{10}$$

$$P(r)=A\{\exp(-3.05r)+0.095\exp(-1.25r)\}r^2. \tag{11}$$

Here the normalization constant A is different from that of the unperturbed wave function A_0, the relation between both constants being

$$A^2=A_0^2\left(1-\frac{1}{3}\bar{r}^2\lambda^2\right). \tag{12}$$

For $2p$-functions of O^{--} ion we shall assume the similar form as (10) with a little different radial part.[5]

$$P(r)=A\{\exp(-2.9r)+0.15\exp(-1.1r)\}r^2. \tag{13}$$

Further, we shall neglect the changes of $2s$-wave function of negative ions and all the wave functions of positive ions, because the polarizability of the positive ions is much smaller than that of the negative ions. The parameter λ in eq. (10) is to be determined by the extremum condition of

$$\partial\Delta E/\partial\lambda=0\,. \tag{14}$$

Now we shall treat below the static case and the high frequency case separately.

§ 3. High frequency field

In this case a polarization of the medium is only due to the polarization of the ions, that is to say, a distortion of their electronic charge distributions. If we take the wave function as eq. (10), ΔE_0 has been given already by Kirkwood as follows:

$$\Delta E_0 = -4\bar{r}^2 F\lambda + 3.0\lambda^2,$$

where the first term gives the energy contribution from the external field F and the second term the change of the kinetic energy due to a distortion of ion. In the present case, however, ions are imbedded in the crystal, so the energy due to the mutual interaction of distorted dipoles has to be added. This energy is according to Fowler

$$-\frac{1}{2}\frac{4\pi}{3}\frac{(4\bar{r}^2)^2}{2a^3}\lambda^2, \tag{15}$$

where a is the interionic distance, $2a^3$ the volume of the unit cell and

$$\bar{r}^2 = \int_0^a |P(r)|^2 r^2 dr, \tag{16}$$

the upper limit of integral being a to allow for the ions imbedded within crystal. Summing these terms we get the energy change ΔE_0 corresponding to the point dipole approximation of Fowler. Namely it follows

$$\Delta E_0 = -4\bar{r}^2 F\lambda - \frac{1}{2}\frac{4\pi}{3}\frac{(4\bar{r}^2)^2}{2a^3}\lambda^2 + 3\lambda^2. \tag{17}$$

When we, however, take accout of the fact that the neighbouring ions overlap to an appreciable extent, eq. (17) has to be modified by additional terms of ΔE_1 and ΔE_2 in (9). First of all, we shall compute the Coulomb interaction between a F^- ion situated at a lattice point and one of the twelve nearest neighbouring F^- ions. When we use the wave function (10) the Coulomb energy consists of the three terms, each of which containing zero, one and two powers of λ respectively. The zero order terms consist of Coulomb interaction among the point charge and its correction terms, which are important for computing the cohesive energy of the crystal but now are dropped off in our problem. The first order terms are cancelled out because of the crystal symmetry in cubic crystals. The second order terms consist of two terms; one is the Coulomb repulsion term of

$$\left(\frac{e^2}{\sqrt{2}a}\right)(1-6\bar{r}^2\lambda^2/3)^2 \approx \left(\frac{e^2}{\sqrt{2}a}\right)(1-4\bar{r}^2\lambda^2) \tag{18}$$

instead of $(e^2/\sqrt{2}a)$, owing to the change of normalization constant A in (12), and the other one is

$$I = \frac{4\lambda^2}{12}\left[-5e^2\left(\frac{3}{4\pi}\right)\int\frac{2|P(r)|^2 r^2\cos^2\theta d\tau_1}{r_{1b}} - 5e^2\left(\frac{3}{4\pi}\right)\int\frac{2|P(R)|^2 R^2\cos^2\theta d\tau_2}{r_{2a}}\right.$$

$$+e^2\left(\frac{3}{4\pi}\right)^2\iint 2|P(r)|^2|P(R)|^2\frac{}{r_{12}}(r^2\cos^2\theta+R^2\cos^2\Theta+2rR\cos\theta\cos\Theta)\,d\tau_1 d\tau_2\Big]$$

$$+\frac{8\lambda^2}{12}\Big[\begin{array}{l}\text{terms obtained by the replacement of } \cos\theta \text{ with } \sin\theta\cos\phi \text{ and}\\ \cos\Theta \text{ with } \sin\Theta\cos\Phi \text{ respectively in the above equations,}\end{array}\Big] \qquad (19)$$

where the origin of the polar coordinates r, θ, ϕ is situated at a central ion and R, Θ, Φ at a neighbouring ion, r_{1b} and r_{2a} are the distance of the electrons from nucleus b and a respectively, and r_{12} the mutual distance of two electrons. After simple calculation, the first and second terms in (19) become,

$$(-5e^2)\left(\frac{3}{4\pi}\right)\int\frac{2|P(r)|^2r^2\cos^2\theta}{r_{1b}}d\tau_1=-10e^2\left(\frac{\bar{r}^2}{\sqrt{2}a}\right)+\text{correction term},$$

$$(-5e^2)\left(\frac{3}{4\pi}\right)\int\frac{2|P(R)|^2R^2\cos^2\Theta}{r_{2a}}d\tau_2=-10e^2\left(\frac{\bar{R}^2}{\sqrt{2}a}\right)+\text{correction term}$$

and the first and second parts involved in the third term of (19) become

$$e^2\left(\frac{3}{4\pi}\right)^2\iint 2|P(r)|^2|P(R)|^2r^2\cos^2\theta/r_{12}d\tau_1 d\tau_2=12e^2(\bar{r}^2/\sqrt{2}a)+\text{correction term},$$

$$e^2\left(\frac{3}{4\pi}\right)^2\iint 2|P(r)|^2|P(R)|^2R^2\cos^2\Theta/r_{12}d\tau_1 d\tau_2=12e^2(\bar{R}^2/\sqrt{2}a)+\text{correction term},$$

where $\bar{r}^2=\bar{R}^2$, the correction terms are given by definite integrals ranging from $2a$ to ∞. The value of such correction terms is estimated to be so small that we are allowed to neglect them in the following computations. In a similar way we may calculate the corresponding terms in the fourth term of (19). Substituting the above results into (19), we get

$$I=\frac{1}{3}\lambda^2\left(\frac{4e^2\bar{r}^2}{\sqrt{2}a}\right)+\frac{2}{3}\lambda^2\left(\frac{4e^2\bar{R}^2}{\sqrt{2}a}\right)$$

$$+\frac{16e^2}{3}\left(\frac{3}{4\pi}\right)^2\lambda^2\iint|P(r)|^2|P(R)|^2rR\cos\theta\cos\Theta/r_{12}\,d\tau_1\,d\tau_2$$

$$+\frac{32e^2}{3}\left(\frac{3}{4\pi}\right)^2\lambda^2\iint|P(r)|^2|P(R)|^2rR\sin\theta\sin\Theta\cos\phi\cos\Phi/r_{12}\,d\tau_1\,d\tau_2. \qquad (20)$$

The sum of the first and second terms of (20) becomes $(4e^2\bar{r}^2/\sqrt{2}a)\lambda^2$, which is cancelled out by the second term of eq. (18). The third and the fourth terms of eq. (20) can be reduced to

$$\frac{16}{3}e^2\lambda^2[-2\bar{r}^2\bar{R}^2/(\sqrt{2}a)^3]+\text{correction term}$$

and

$$\frac{32}{3}e^2\lambda^2[\bar{r}^2\bar{R}^2/(\sqrt{2}a)^3]+\text{correction term}$$

respectively.

The first terms of the above expressions represent effectively the electrostatic interaction between point dipoles, which are cancelled out for NaCl type crystal, whereas the correction terms are caused by the overlapping of the charge clouds, being expressed by

$$\int_0^\infty |P(r)|^2 r dr \int_{\sqrt{2}a-r}^{\sqrt{2}a+r} \left[\begin{array}{l}\textit{algebraic function of}\\ r,\ a\ \textit{and}\ r_{1b}\end{array}\right] e^{-2\beta r_{1b}} dr_{1b}.$$

The algebraic function in the integrand is so lengthy that we are compelled to compute by numerical integration. Here we neglect the deformation of Li^+ ion for the reason mentioned above.

Next we shall compute the change of the exchange energy between F^- and Li^+ ion caused by the deformation of $2p$- wave function of the former. In accordance with the method of Landshoff,[6] the integral C_L, named by him, takes the followingfor m in our case,

$$C_L = \iint [\Psi_0(r_1)(1+\lambda r_1 \cos\theta_1)\phi_{Li}(r_1)\Psi_0(r_2)(1+\lambda r_2\cos\theta_2)\phi_{Li}(r_2)]/r_{12} d\tau_1 d\tau_2. \quad (22)$$

This integral also consists of the terms, each containing zero, one and two powers of λ respectively. The zero order term is important for the cohesive energy, which is dropped off in our problem. The first order terms are cancelled out by crystal symmetry, when allowing for the contributions from six nearest neighbours. The second order terms are computed by the method similar to the zero order term, but the former is less accurate than the latter, due to the larger overlapping of the wave functions. We may also compute the integral B_L in Landshoff theory in the similar way. Next we have to compute the change of the exchange energy between F^- ion and F^- ion. The method is quite similar to the above. Thus we get all the correction terms, denoted by $A\lambda^2$, to (17)

$$\Delta E = -4\bar{r}^2 F\lambda - \frac{1}{2}\frac{4\pi}{3}\frac{(4\bar{r}^2)^2}{2a^3}\lambda^2 + 3\lambda^2 + A\lambda^2. \quad (23)$$

By the use of (23), the extremum condition (14) leads to

$$\lambda = 4\bar{r}^2 F \Big/ \left[2(A+3) - \frac{4\pi}{3}\frac{(4\bar{r}^2)^2}{2a^3}\right]. \quad (24)$$

Inserting (24) into (23) the required value of ΔE is given by

$$\Delta E = -\left\{(4\bar{r}^2)^2 \Big/ 2\left[2(3+A) - \frac{4\pi}{3}\frac{(4\bar{r}^2)^2}{2a^3}\right]\right\} F^2. \quad (25)$$

Then we may obtain the dielectric constant $\varkappa_0$ by the relations:

$$\Delta E = -\frac{1}{2}\chi_0 F^2, \qquad \varkappa_0 = 1 + 4\pi\chi_0/2a^3. \quad (26)$$

The effective field F_{eff}, therefore, becomes

$$F_{eff} = F + \frac{4\pi}{3}P = \left\{2(3+A) \Big/ \left[2(3+A) - \frac{4\pi}{3}\frac{(4\bar{r}^2)^2}{2a^3}\right]\right\} F, \quad (27)$$

and the polarizability α, through the relation

$$4\bar{r}^2\lambda=\alpha F_{eff}, \tag{28}$$

and obtained

$$\alpha=(4\bar{r}^2)^2/2(3+A). \tag{29}$$

§ 4. Numerical results and discussion

The numerical results for LiF and MgO, using the atomic unit, shall be presented in the following.

(1) LiF:

Using the calculated values of $\bar{r}^2=1.90$, $A=0.80$, and the observed one of $\alpha=3.78$, we obtain

$$\begin{aligned}\Delta E&=-7.60F\lambda-1.11\lambda^2+3\lambda^2+0.80\lambda^2 \qquad (30)\\ &=-7.60F\lambda+2.69\lambda^2\end{aligned}$$

for (23) and

$$\lambda=1.41F \qquad (30')$$

for (24), which leads to

$$\Delta E=-\frac{1}{2}(10.7)F^2, \qquad \chi_0=10.7$$

and

$$\varkappa_0=2.33.$$

The effective field $\boldsymbol{F}_{eff}$, (27), becomes $\boldsymbol{F}_{eff}=1.41F$, then we obtain the following value for polarizability of F^- ion $\alpha=1.08\times10^{-24}$ (c.g.s. unit), whereas Shockley's value of α[7] is: $\alpha=0.86\times10^{-24}$, and the observed value of $\varkappa_0$ is 1.92.

Our calculated $\varkappa_0$ value is seen to become larger in comparison with the observed one, which discrepancy is considered to be caused mainly by our less accurate value of A and the approximate nature of the unperturbed wave functions, though our calculated value, $\bar{r}^2=1.90$, is in good accordance with the observation. On the whole we may say our theory is in the rather good accordance with the observation, as far as the approximate nature of our method is taken into consideration.

(2) MgO:

Using the calculated values of $\bar{r}^2=3.19$, $A=1.9$ and the observed one of $\alpha=4.0$, we obtain

$$\Delta E=-12.66F\lambda+2.55\lambda^2, \qquad (31)$$

$$\lambda=2.83F, \quad \therefore\ \Delta E=-\frac{1}{2}(36.1)F^2,$$

and

$$\chi=36.1,$$

then

$$\varkappa_0=4.56.$$

The observed value for MgO is $\varkappa_0=2.95$.

Our calculated value is larger than the observed value by about 50%, which may be caused mainly by the inaccuracy of our unperturbed wave function (13). On determining this wave function by the variational method, we have neglected the interaction energy between the O^{--} ion and its next-nearest twelve O^{--} ions, which neglection may perhaps result in the rather large spreading of the charge distribution of O^{--} ion. Actually we obtained the calculated value of -24.7×10^{-6} for diamagnetic susceptibility of MgO crystal, while the observed one is of only -18.8×10^{-6}, which fact seems to justify the above consideration.

Now we see, from eq. (30) and eq. (31), that the energy contribution from the Lorentz factor is almost cancelled out by the energy contribution resulting from the change of the exchange and dipole interaction energies. Although we may not give a precise classical interpretation to the energy caused mainly by exchange interaction, we may be allowed to interpret it phenomenologically as follows.

At first we may suppose the Lorentz equation is valid within the crystal, but the polarizability of the negative ion is reduced to $(4\bar{r}^2)^2/2(3+A)$ in the crystal instead of $(4\bar{r}^2)/6$ in free state. In practice we may choose a suitable value for polarizability of each ion in the crystal so as to give a correct value of the dielectric constant; such phenomenological treatment has been performed by Shockley.[7] Alternatively we may think the polarizability of the ions in a free state remains unchanged within the crystal but the Lorentz equation is no more valid within the crystal on account of the contribution from the Lorentz factor being almost cancelled out by $A\lambda^2$. Such viewpoint corresponds to Mott's eq. (5).

§ 5. Static case

Let us consider here a crystal in equilibrium under the influence of a static field F. In equilibrium the positive and negative ions will displace by the amount of $\pm x$ from their mean positions, and let the dipoles induced on the negative ions be $4\bar{r}^2e\lambda$. Now we shall consider the case of LiF crystal, in which the polarizability of the positive ions will be neglected. When the crystal is polarized, we may imagine that the negative ions remain in their original positions, while the positives are displaced a distance $2x$. Then energy change of a ion-pair is as follows:

(1) the energy due to the ionic displacement in the external field:

$$-2exF, \tag{32}$$

(2) the mutual interaction energy of the dipoles with moment $2ex$:

$$-\frac{1}{2}\frac{4\pi}{3}\frac{(2ex)^2}{2a^3}, \tag{33}$$

(3) the deformation energy of the ion-core of a negative ion in the external field:

$$4\bar{r}^2e\lambda F, \tag{34}$$

(4) the mutual interaction energy of the dipoles with moment $4\bar{r}^2e\lambda$:

$$-\frac{1}{2}\frac{4\pi}{3}\frac{(4\bar{r}^2e)^2}{2a^3}\lambda^2, \tag{35}$$

(5) the mutual interaction energy between a dipole of $2ex$ and a dipole of $4\bar{r}^2e\lambda$:

$$-\frac{4\pi}{3}\frac{(2ex)(4\bar{r}^2e\lambda)}{2a^3}. \tag{36}$$

Summing them and differentiating by $2x$ or λ, we obtain for the effective field,

$$F_{eff}=F+\frac{4\pi}{3}\frac{2ex}{2a^3}+\frac{4\pi}{3}\frac{4\bar{r}^2e\lambda}{2a^3}=F+\frac{4\pi}{3}P. \tag{37}$$

(6) Next we have to find the repulsive energy, from which the restoring force on each ion is derived. If the repulsive potential is assumed to be effective only among the nearest neighbouring ions and be expressed by

$$W(r)=A\exp(-r/\rho), \tag{38}$$

we obtain the repulsive energy of the following form

$$px^2=\frac{2\alpha_M e^2}{3a^2}\left[\frac{1}{\rho}-\frac{2}{a}\right]x^2, \tag{39}$$

where α_M is the Madelung constant. Using the compressibility β which satisfies

$$\frac{1}{\beta}=\frac{e^2}{9a^2}\frac{\alpha_M}{2}\left[\frac{1}{\rho}-\frac{2}{a}\right], \tag{40}$$

we may determine p in (39) empirically through the following relation

$$p=12a/\beta\,. \tag{41}$$

(7) Further we have to consider the term $A\lambda^2$ as § 4.

(8) In § 4, when the ions are not displaced, the first order term of λ in exchange energy (22) have not been considered, because the contributions from the two positive ions, situated at symmetrical positions of a negative ion, are cancelled out by symmetry.

In the static field, two positive ions are displaced, one is situated at $a+2x$, while the other at $a-2x$ from the negative ion, then the first order terms of λ are no more cancelled out, but the difference of the type $B\lambda x$ remains, where B is the exchange integral contained in C_L (22) and B_L. We assume B may also take a form $b\exp(-qr)$ for interionic distance r. In practice we have computed numerically the exchange energy by Landshoff's method for two points near the distance $a=3.78$ and determine the constants b and q from these values.

Summing up all the energy contributions of different origins mentioned above, we have obtained the total energy as follows :

$$\Delta E=-2exF-\frac{1}{2}\frac{4\pi}{3}\frac{(2ex)^2}{2a^3}-\frac{4\pi}{3}\frac{(2ex)(4\bar{r}^2e\lambda)}{2a^3}-4\bar{r}^2eF\lambda$$

$$-\frac{1}{2}\frac{4\pi}{3}\frac{(4\bar{r}^2e\lambda)^2}{2a^2}+\frac{2\alpha_M e^2}{3a^2}\left[\frac{1}{\rho}-\frac{2}{a}\right]x^2+3\lambda^2+A\lambda^2+B\lambda x. \tag{42}$$

According to the variational principle, λ and x can be determined by the conditions

$$\partial\Delta E/\partial\lambda=0, \qquad \partial\Delta E/\partial x=0. \tag{43}$$

§ 7. Results

From the compressibility data of LiF, we find the extrapolated value at 0°K of β to be 1.4×10^{-12} (c.g.s.) and from (41) p becomes 0.111 in atomic unit. The computed value of $Bx\lambda$ is

$$B\lambda x=(2\lambda)(0.034)\left[e^{1.85(2x)}-e^{-1.85(2x)}\right]=0.503\lambda x.$$

Then ΔE in atomic unit (cf. eq. (42)) becomes

$$\Delta E=-2xF-0.077x^2-0.587x\lambda-7.6\lambda F-1.10\lambda^2$$
$$+0.111x^2+3\lambda^2+0.80\lambda^2+0.503\lambda x. \tag{44}$$

From (43) we may determine x and λ,

$$x=16.64\lambda, \quad \lambda=1.91F, \qquad x=31.8F. \tag{45}$$

Using these values, ΔE, χ and $\varkappa$ become

$$\Delta E=-39.0F, \qquad \chi=78 \quad \text{and} \quad \varkappa=10.1$$

respectively. The observed value for this is: $\varkappa=9.3$.
The agreement is quite good, as far as the approximate nature of our method is taken into account.

As far as our approximate calculation concerns, the polarization energy due to the deformation of the ion-core (35) is almost cancelled out by $A\lambda^2$, and the coupling energy (36) of two types of polarization is also almost cancelled out by $Bx\lambda$. These facts may be interpreted as follows: If we consider $A\lambda^2$ as a sort of a restoring energy like $3\lambda^2$, and $Bx\lambda$ also as a restoring energy like px^2, so we may say the effective field is still given by the Lorentz field as in eq. (37). On the other hand if we consider only the terms $3\lambda^2$ and px^2 as the restoring energy but not $A\lambda^2$ and $Bx\lambda$, so we may lead to the conclusion that the effective field for displaced ion is

$$F_{eff}=F+\frac{4\pi}{3}\frac{2ex}{2a^3}+\frac{4\pi}{3}\gamma\frac{4\bar{r}^2e\lambda}{2a^3}=F+\frac{4\pi}{3}P_i+\frac{4\pi}{3}\gamma P_e \tag{46}$$

and the effective field, which gives rise to the deformation of the ion-core is

$$F'_{eff}=F+\frac{4\pi}{3}\gamma P_i+\frac{4\pi}{3}\gamma' P_e. \tag{47}$$

In the case of LiF we have seen $\gamma \sim 0$ and $\gamma' \sim 0$.

The meaning of Mott's equation (5) corresponds to the second interpretation. We, however, should like to point out that these interpretations are rather phenomenological, because the terms $A\lambda^2$ and $Bx\lambda$ are mainly due to the exchange energy.

§ 8. The effective charge

As seen above, when the ions are displaced in static field, the apparent restoring force is added to the usual one so as to hinder the deformation of the ion-core. When we may interpret this fact as the apparent decrease of polarizability of each ion, it will be misleading to separate the total polarization $\boldsymbol{P}$ into the ionic polarization $\boldsymbol{P}_i$ and the electronic polarization $\boldsymbol{P}_e$, $\boldsymbol{P}_e$ taking the same value as that of optical case. Recently Fröhlich[8] has worked out this problem phenomenologically, separating $\boldsymbol{P}$ as $\boldsymbol{P}=\boldsymbol{P}_0+\boldsymbol{P}_{ir}$ instead of $\boldsymbol{P}=\boldsymbol{P}_e+\boldsymbol{P}_i$, where $\boldsymbol{P}_0$ is the optical polarization and $\boldsymbol{P}_{ir}$ is the infra-red polarization due in part to the redistribution of electron which results directly from the change in position of the ions. Then he has put

$$P_{ir}=2xe^*N \tag{48}$$

using the effective charge e^* for the true charge e and determined e^* from a set of the experimental values. Let us here derive e^* from our theory. From the relations $\boldsymbol{P}=\boldsymbol{P}_0+\boldsymbol{P}_{ir}=\boldsymbol{P}_e+\boldsymbol{P}_i$ and $\boldsymbol{P}_{ir}=e^*\boldsymbol{P}_i$, we obtain

$$P_0=P_e+(1-e^*)P_i\,. \tag{49}$$

On the other hand, we have the relation

$$P_0/N=a\left[F+\frac{4\pi}{3}P_e+\frac{4\pi}{3}P_i\right]. \tag{50}$$

From (49), (50) and the definitions of $\boldsymbol{P}_e$ and $\boldsymbol{P}_i$ we obtain

$$4\bar{r}^2\lambda+(1-e^*)2x=a\left[F+\frac{4\pi}{3}\frac{4\bar{r}^2}{2a^2}\lambda+\frac{4\pi}{3}\frac{2x}{2a^3}\right]. \tag{51}$$

Inserting the values of λ, x and a into (51), we have for the value of e^* : $e^*=0.76$, which value is in good accordance with the Fröhlich's value of $e^*=0.83$.

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References

1) Mott-Gurney, *Electronic Processes in Ionic Crystals*, Chap. I.
2) Hasse, Proc. Camb. Phil. **26** (1930), 542.
3) J. C. Slater, and J. G. Kirkwood, Phys. Rev. **37** (1931), 682.
J. G. Kirkwood, Phys. ZS. **33** (1932), 57.
4) J. Yamashita, J. Phys. Soc. Jap, **7** (1952), 284.
5) J Yamashita and M. Kojima, J. Phys. Soc. Jap. **7** (1952), 261.
6) R. Landshoff, ZS. f. Phys. **102** (1936), 201.
7) W. Shockley, Phys. Rev. **70** (1946), 105.
8) H. Fröhlich, *Theory of Dielectrics* (1949), § 18.

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On Equivalent Observers

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In the present paper we investigate the nature of equivalent observers (hereafter to be designated as E.O.). The idea of E.O. is very important in relativistic theory. As a result of this investigation it is found that we must introduce a new idea of E.O. different from the E.O. hitherto employed to treat various phenomena in physics. First we show the existence of two kinds of E.O. in our sense and then study their properties briefly.

§ 1. Introduction

The concept of the equivalency of observers is one of the most important ideas in relativistic theories. In fact, the principle of special relativity is nothing but the assertion of the equivalency for observers moving uniformly relative to each other, and the principle of covariance in general relativity is simply that of equivalency for all observers moving arbitrarily relative to each other, though the meanings of the term " equivalency " used in both cases are not the same. Also, it is well known that Milne's " Kinematic relativity " is based on his excellent idea concerning E.O.[1)]

We shall at first analyse the properties of E.O. commonly used. This analysis leads us to introduce a new concept of E.O. different from those hitherto used (§ 2). Next the properties of coordinate transformations between these E.O. are investigated and the characters of equivalency of physical laws under these transformations are studied (§ 3). An example of the method to determine such E.O. is shown in § 4. After that, two kinds of E.O. are obtained by this method, their properties are studied briefly and the explicit forms of the coordinate transformations between E.O. are obtained. In this manner it is found that Lorentz transformation, Sibata's transformation in wave geometry, Page's transformation in his " New relativity ", etc. are contained as special cases in our transformations.

§ 2. Equivalent observers

In general relativity which is based on the principle of covariance, any physical law must have an invariant meaning under any coordinate transformation. Thus it is required, in general relativity, that all physical quantities are represented by the tensor quantities which preserve definite meanings under any coordinate transformation and that the physical laws must be expressed as the tensor equations concerning these quantities. Therefore the general

theory of relativity is the most general one from the standpoint of the equivalency of the observers. But the idea of the covariancy of the physical laws in this theory is so comprehensive that it even requires its validity for the coordinate transformations of no physical meaning.

In this paper we intend to investigate the equivalency of observers connected by the transformations which correspond to physical reality. Lorentz transformation in special relativity is indeed one of these transformations, but as is easily seen, it is impossible to treat all physical phenomena in the scope of special relativity. For example, this theory is not applicable to the phenomena in the presence of a large mass. Also it is not unquestionable whether we can apply the idea of E.O. in quantum physics just as in classical physics, since, for instance, the quantum mechanical disturbance is caused by the observation. Moreover, it is not ensured perfectly that we can represent the whole features of the quantum mechanical objects by using only Lorentz invariant concepts. For example, if we try to describe the inner structures of elementary particles using some non-local model (in the widest sense), a question arises whether Lorentz invariance is required for such model, or not.

Therefore it is desirable to construct new theories appropriate for the physical phenomena which cannot be treated either in special or general relativity. For this reason we shall first change the concept of the E.O. into a new one. In ordinary theories it is required that the E.O. have the equivalency for all physical laws. As is mentioned above, however, it is not without doubt to believe that there exist the observers which have such wide equivalency. Hereafter we shall only deal with such E.O. that are equivalent with each other with respect to "some", instead of "all", definite physical laws.

§ 3. Coordinate transformation between equivalent observers

It seems valuable to examine the situation of Lorentz transformation in special relativity before we study the problem of coordinate transformation between E.O. in the new sense. In the special theory of relativity, though observers moving uniformly relative to each other are equivalent, mathematical expressions of the physical laws for such observers are not the same if they choose their space-time coordinates arbitrarily and independently of each other (e.g. if one takes cartesian coordinate and another takes polar coordinate for the space-frame), because the laws are not invariant under such general transformations. Only when each observer uses the coordinate in which $ds^2 = -dx^2 - dy^2 - dz^2 + c^2 dt^2$ holds the mathematical expressions are invariant (more precisely, form-invariant) under the Lorentz transformation of ordinary form.

The idea of the form-invariancy of mathematical expressions was studied in detail first in relativistic cosmology with respect to the metric of the space-time.[2] Now we shall use it not only for metric but also for physical laws of interest. Then every E.O. must take a space and time coordinate system of the same kind so that the coordinate variables may have the same meaning in each system, otherwise the requirement of the form-invariancy of the physical laws should have no meaning.

Now we shall study the characteristic features of these transformations. Firstly from our new definition of equivalency it seems natural to assume that the transformations form a group $\mathfrak{G}$ just as Lorentz transformations in a wide sense form the full Lorentz group.

Next we shall examine the converse problem: whether or not we can define E.O. when a group $\mathfrak{G}$ of coordinate transformations is given previously. In general we can find some invariant relations under $\mathfrak{G}$, then the physical laws to be defined by $\mathfrak{G}$ must be expressed by these invariant relations. If the elements of $\mathfrak{G}$ have real physical meaning, we can consider that the observers connected by the elements of $\mathfrak{G}$ have physical reality. In this case we can define E.O. connected by the elements of $\mathfrak{G}$.

Consequently we can conclude as follows. We assume that transformations between E.O. form a group $\mathfrak{G}$. And then we do not regard the set of observers as equivalent when the transformations connecting these observers do not form a group. When the relative motions of the coordinate systems connected by the elements of any given $\mathfrak{G}$ correspond to physical reality, we can define E.O. Therefore we have the following two ways to construct the theory of E.O.:

(i) *When the physical laws for which the form-invariancy is required are known previously, we have only to search for the transformations which keep the mathematical expressions of these laws form-invariant,*

(ii) *When the transformation group $\mathfrak{G}$ is given previously, we have only to determine the invariant relations under $\mathfrak{G}$ by which the physical laws are defined.*

The main contents of the following are to determine the group of coordinate transformations connecting E.O. by using the latter way (ii).

§ 4. Postulates for equivalent observers

In the following sections we shall define two kinds of E.O. and investigate their properties. For this purpose we shall study the structure of the group formed by the transformations connecting these observers.

At first we shall examine the properties of the elements of $\mathfrak{G}$. We can classify these elements according to the relative motions between coordinate systems as follows:

(a) Transformations between coordinate systems which are relatively *at rest.*

(b) „ „ „ „ *in motion.*

Hereafter we call a transformation belonging to (a) the frame-transformation. We shall assume that any frame-transformation is the coordinate transformation between the coordinate systems employed by the same observer and vice versa. Then any transformation belonging to (b) can be regarded as transformation between coordinate systems employed by different observers and vice versa.

Now, if there is a set of frame-transformations which form a group $\mathfrak{G}_0$, in general we can find some physical laws form-invariant under this group. In this case we shall say that "the systems connected by this $\mathfrak{G}_0$ are equivalent with respect to these laws." Then if there are some transformations connecting different observers which also keep form-invariant the mathematical expressions of these laws, they must form an enlarged group

together with the given frame-transformations.

Therefore we shall first assume the form of the group $\mathfrak{G}_0$ and then shall proceed to construct the whole group $\mathfrak{G}$ by using some suitable postulates. In the following we shall deal with two kinds of E.O. whose $\mathfrak{G}_0$ are given by (i) the group composed of the motions in three dimensional Euclidean space and the translation of time, and (ii) the group of the three dimensional rotations. We shall call these two kinds of observers *the E.O. of the first kind* and *the E.O. of the second kind* respectively.

Now we shall give our postulates for E.O. of the first kind. We shall start with :

(P.I) *Any "E.O." M is furnished with a three dimensional "space-frame" S with origin M and a one dimensional "time-frame" T, and can give one and only one set of space coordinates (x,y,z) and time coordinate (t) to any "point event" E to within frame-transformations.*

By this postulate the observation of E by M is simply that M gives one and only one set of four real variables (i.e. coordinates (x,y,z,t)) to E. Here, we shall not touch on the problem of observation, i.e. "How we can make one to one correspondence between E and (x,y,z,t)?", though it is a very important problem in physics.

Let M and M' be any observers, and E any event. If (x^i) and (x'^i), where $i=1,\ldots,4$ and $x,y,z,t \equiv x^1,\ldots,x^4$, are coordinates of E given by M and M', we have

$$x'^i = f^i(x^j), \quad |\partial x'^i/\partial x^j| \neq 0, \quad (i,j=1,\ldots,4), \tag{4·1}$$

from (P.I).

(P. II) *Any observer M can observe all other E.O. and they are moving relative to M.*

Hence there are no E.O. at rest relatively to each other.

(P. III) *The group of frame-transformations $\mathfrak{G}_0$ is given by*

the rotations $$R_1 = z\partial_y - y\partial_z, \quad R_2 = x\partial_z - z\partial_x, \quad R_3 = y\partial_x - x\partial_y \tag{4.2}$$

and the translations $$T_1 = \partial_x, \quad T_2 = \partial_y, \quad T_3 = \partial_z \tag{4.3}$$

of space-frame S_M of M, and the translation $$U = \partial_t \tag{4.4}$$

of time-frame T_M of M. And this $\mathfrak{G}_0$ forms a continuous group of transformations together with the set of transformations given by (4·1).

In ordinary words this postulate corresponds to the fact that the space-frame of M is isotropic and homogeneous and time-frame of M is homogeneous from the standpoint of the group $\mathfrak{G}$.

(P. IV) *If M and M' are any two E.O. they make radial motions relative to each other and, furthermore, if M observes any E on the straight line MM', then M' also observes the E on the straight line $M'M$ independent of each time coordinate t and t'.*

In this postulate the "straight line" means the set of all points invariant under any rotation of S_M. Hence its analytical expression is the same as that in ordinary Euclidean geometry.

These are the whole postulates which we put for our E.O. of the first kind. If we take Lorentz transformation or Galilean transformation as (4.1) the four postulates are all

satisfied. But the contrary is not necessarily the case. These circumstances are made clear in due course.

§ 5. Analytical expressions of the postulates

In this section we shall give the analytical expressions of the postulates for our set of E.O. of the first kind given in the last section and shall obtain the equations which we have to solve in order to determine $\mathfrak{G}$.

Let M and M' be two arbitrary E.O. From (P. III), we can take x_M-axis (i.e. $y_M=z_M=0$) so that M' lies on it by making suitable rotation of S_M. Then by (P. IV) M' moves on x_M-axis relative to M. Similarly we can rotate $S_{M'}$ so that M moves on $x_{M'}$-axis relative to M'. If we assume that M and M' are infinitesimally near, (4.1) becomes an infinitesimal transformations. Let

$$P_1=\alpha(x,y,z,t)\partial_x+\beta(x,y,z,t)\partial_y+\gamma(x,y,z,t)\partial_z+\delta(x,y,z,t)\partial_t \tag{5.1}$$

be its symbol. Of course $\alpha,\ldots,\delta$ are assumed to be regular in the domain of interest and their partial derivatives to be finite at $x=y=z=0$ and $t=t$ as in ordinary theory of continuous group. From (P. IV), we have

$$\beta(x,0,0,t)=\gamma(x,0,0,t)=0, \quad \alpha(0,0,0,t)\neq\text{const.}, \text{ so } \alpha(0,0,0,t)\neq 0. \tag{5.2}$$

Denoting the rotation $x'=y$, $y'=z$, $z'=x$ by R_0 and putting $P_2=R_0^{-1}P_1R_0$ and $P_3=R_0^{-1}P_2R_0$, we have

$$P_2=\gamma(y,z,x,t)\partial_x+\alpha(y,z,x,t)\partial_y+\beta(y,z,x,t)\partial_z+\delta(y,z,x,t)\partial_t$$

and

$$P_3=\beta(z,x,y,t)\partial_x+\gamma(z,x,y,t)\partial_y+\alpha(z,x,y,t)\partial_z+\delta(z,x,y,t)\partial_t. \tag{5.3}$$

Evidently P_2(or P_3) gives the transformation between M and its neighbouring observer M'' (or M''') situated on the y_M(or z_M)-axis of S_M. Combining these transformations we can obtain the transformation between M and its neighbouring M_1 in any direction relative to M. The postulate (P. III), accordingly, becomes the requirement that ten operaters

$$\mathfrak{G}\ :\ R_1,R_2,R_3;\quad T_1,T_2,T_3;\quad U;\quad P_1,P_2,P_3 \tag{5.4}$$

form the group $\mathfrak{G}$. As is well known, the following relations hold for the sub-group of frame-transformations $\mathfrak{G}_0$:

$$\begin{gathered}(R_a,R_b)=\epsilon^{abc}R_c,\quad (T_a,T_b)=0,\quad (R_a,T_b)=\epsilon^{abc}T_c,\\ (R_a,U)=0,\quad (T_a,U)=0,\quad (a,b,c=1,2,3),\end{gathered} \tag{5.5}$$

where ϵ^{abc} is antisymmetric in all indices with $\epsilon^{123}=1$, and summation convention is used.

A necessary and sufficient condition that (5.4) form the group $\mathfrak{G}$ is that the Poisson operators (U,P_a), (T_a,P_b) and (P_a,P_b) be linear combination (with constant coefficients) of (5.4). Hence to determine $\mathfrak{G}$ we have only to solve these equations.

§ 6. Concrete forms of P_a

As is easily seen, we can obtain

$$(T,P_1)=\dot{\alpha}(x,y,z,t)\partial_x+\dot{\beta}(x,y,z,t)\partial_y+\dot{\gamma}(x,y,z,t)\partial_z+\dot{\delta}(x,y,z,t)\partial_t, \tag{6.1}$$

$$\begin{cases}(T_1,P_1)=(\partial_x\alpha_1)\partial_x+(\partial_x\beta_1)\partial_y+(\partial_x\gamma_1)\partial_z+(\partial_x\delta_1)\partial_t,\\ (T_1,P_2)=(\partial_x\gamma_2)\partial_x+(\partial_x\alpha_2)\partial_y+(\partial_x\beta_2)\partial_z+(\partial_x\delta_2)\partial_t,\\ (T_1,P_3)=(\partial_x\beta_3)\partial_x+(\partial_x\gamma_3)\partial_y+(\partial_x\alpha_3)\partial_z+(\partial_x\delta_3)\partial_t,\end{cases} \tag{6.2}$$

$$\begin{cases}(R_1,P_1)=(R_1\alpha_1)\partial_x+(R_1\beta_1-\gamma_1)\partial_y+(R_1\gamma_1+\beta_1)\partial_z+(R_1\delta_1)\partial_t,\\ (R_1,P_2)=(R_1\gamma_2)\partial_x+(R_1\alpha_2-\beta_2)\partial_y+(R_1\beta_2+\alpha_2)\partial_z+(R_1\delta_2)\partial_t,\\ (R_1,P_3)=(R_1\beta_3)\partial_x+(R_1\gamma_3-\alpha_3)\partial_y+(R_1\alpha_3+\gamma_3)\partial_z+(R_1\delta_3)\partial_t,\end{cases} \tag{6.3}$$

$$(P_1,P_2)=(P_1\gamma_2-P_2\alpha_1)\partial_x+(P_1\alpha_2-P_2\beta_1)\partial_y+(P_1\beta_2-P_2\gamma_1)\partial_z+(P_1\delta_2-P_2\delta_1)\partial_t \tag{6.4}$$

and those obtained from these relations by cyclic change of x, y and z, where a dot means derivative with respect to t and $\alpha_1=\alpha(x,y,z,t)$, $\alpha_2=\alpha(y,z,x,t)$, $\alpha_3=\alpha(z,x,y,t)$, etc. Next, by putting these Poisson operators as linear combinations with constant coefficients of R_a, T_a, U and P_a, we have 24 sets of simultaneous equations. Each of these sets is composed of four partial differential equations of the first order containing ten undetermined constant coefficients. For example, the sets obtained from the third of (6.3) is given by

$$\begin{aligned}&R_1\beta_3=a\alpha_1+b\gamma_2+c\beta_3-fz+gy+l,\\ &R_1\gamma_3-\alpha_3=a\beta_1+b\alpha_2+c\gamma_3-gx+ez+m,\\ &R_1\alpha_3+\gamma_3=a\gamma_1+b\beta_2+c\alpha_3-ey+fx+n,\\ &R_1\delta_3=a\delta_1+b\delta_2+c\delta_3+p,\end{aligned} \tag{6.5}$$

where $a,b,c,\ldots,p$ are undetermined constants.

Using the relation $\alpha(0,0,0,t)\neq 0$ which is obtained from (5.2), and the equations obtained from (6.1), (6.2) and (6.3), we have the following relations:

$$\alpha_1=x^2\rho+\tau,\ \beta_1=xy\rho+z\theta,\ \gamma_1=xz\rho-y\theta,\ \delta_1=x\sigma+p, \tag{6.6}$$

where ρ,τ,θ and σ are arbitrary functions of $r\equiv\sqrt{(x^2+y^2+z^2)}$ and t, and p is an arbitrary constant. (We shall omit the details and give only the outline of the calculations). Then by rewriting P_1-pU as P_1 anew and using the remaining conditions we have:

$$\tau=at+q,\ \theta=q',\ \sigma=b,\ \rho=0, \tag{6.7}$$

in the case of $\sigma\neq 0$, where $a(\neq 0)$, $b(\neq 0)$, q and q' are arbitrary constants. Rewriting $P_1-qT_1-q'R_1$ as P_1 again, we have $\tau=at$, $\theta=0$ and $\sigma=b(a,b\neq 0)$. When $\sigma=0$, in the same way, we have $\tau=\exp(at)$ and $\theta=\sigma=\rho=0$.

Summarizing the results we have:

Theorem 1. *The most general form of P_1 in order that R_a, T_a, U and P_a form a group is given by the following three types to within the transformations of $\mathfrak{G}_0$ (i.e.*

frame-transformations) :

[a] $P_1=t\partial_x+ax\partial_t$, (*a being a const.* $\neq 0$).

In this case, it follows that

$$(P_a,P_b)=a\epsilon^{abc}R_c,\ (R_a,R_b)=\epsilon^{abc}P_c,\ (U,P_a)=T_a,\ (T_a,P_b)=a\delta_{ab}U.$$

[b] $P_1=t\partial_x$.

In this case, it holds that

$$(P_a,P_b)=(T_a,P_b)=0,\quad (R_a,P_b)=\epsilon^{abc}P_c,\quad (U,P_a)=T_a.$$

This type is obtained from [a] *by putting* $a=0$.

[c] $P_1=\exp(at)\partial_x$, (*a being a const.* $\neq 0$).

In this case, it holds that

$$(P_a,P_b)=(T_a,P_b)=0,\quad (R_a,P_b)=\epsilon^{abc}P_c,\quad (U,P_a)=aP_a.$$

It must be noted that in case of [a] P_1, P_2 and P_3 cannot form a sub-group of $\mathfrak{G}$ by themselves alone. This situation also holds for Lorentz transformations i.e. three transformations $L_1=t\partial_x+(x\partial_t)/c^2$, $L_2=t\partial_y+(y\partial_t)/c^2$ and $L_3=t\partial_z+(z\partial_t)/c^2$ in x-, y- and z-directions respectively cannot form a group by themselves. They only form a group together with R_a.[3]

From the standpoint of E.O. theorem 1 can also be expressed in the following way : Theorem 1′. *The most general transformation of coordinates between two E.O. M and M′ satisfying our postulates is given by the three types in the theorem 1 provided we rotate* S_M *and* $S_{M'}$ *so that the straight line MM′ coincides with x-axes of both space-frames.*

Now, we can easily obtain the following finite form of three transformations :

[a′] : $x'=\dfrac{x-Vt}{\sqrt{(1-aV^2)}},\quad y'=y,\ z'=z,\quad t'=\dfrac{t-aVx}{\sqrt{(1-aV^2)}},$

[b′] : $x'=x-Vt,\quad y'=y,\quad z'=z,\quad t'=t,$

[c′] : $x'=x-V\exp(at),\quad y'=y,\quad z'=z,\quad t'=t,$

where V's are the parameters of the transformations.

In each case if we regard (x,y,z) as cartesian coordinates as usual we may interpret the three transformations as follows :

[a′] : This transformation was obtained by Ignatowsky and by Frank-Rothe from another standpoints.[4] When $a=1/c^2$, it becomes Lorentz transformation and when $a\neq 1/c^2$ its physical meaning has not yet been determined.

[b′] : This is nothing but Galilean transformation.

[c′] : In this case, as in [b′], there exists universal time. Relative velocity of the E.O. (i.e. the origins of the coordinate systems connected by this transformation) is proportional to their relative distance :

$$[dx/dt]_{x'=0}=a[x]_{x'=0}. \tag{6.8}$$

Therefore if we take this a as Hubble's constant tentatively, the relative motions of the observers satisfy Hubble's velocity-distance relation concerning nebulae. As is well known, however, in order to investigate the problem of the Hubble's relation we must establish a theory concerning the propagation of light. Here we cannot enter into this problem further. But it may not be meaningless to compare the properties of this transformation with those of Milne's theory in t-measure.[1] Main differences are as follows: (i) In his theory there exists no universal time in t-measure contrary to our case.* (ii) Natural origin of time (i.e. the time of coincidence of the observers) is $t=0$ in his theory, while $=-\infty$ in our case. (iii) The proportional factor corresponding to Hubble's constant is $1/t$ in his theory, while pure constant a in our theory.

§ 7. ds^2 form-invariant under $\mathfrak{G}$

In § 2 we required the form-invariancy of the physical laws for E.O. From this point of view, if we introduce four dimensional Riemannian metric in our space and time, we may consider the form-invariancy of the metric. Hence in the following we shall determine the four dimensional Riemannian space V_4 whose metric is form-invariant under the group $\mathfrak{G}$. Group theoretically, this problem is to determine V_4, which admits $\mathfrak{G}$ as its group of motions. Now, as is well known, the condition that V_4 admits $X=\xi^i\partial_i$ as a motion is given by Killing's equation

$$\xi^k\frac{\partial g_{lm}}{\partial x^k}+\frac{\partial \xi^k}{\partial x^l}g_{km}+\frac{\partial \xi^k}{\partial x^m}g_{lk}=0, \quad (i,j,\ldots=1,\ldots,4), \tag{7.1}$$

where g_{lm} is the fundamental tensor of the V_4.

If we use R_a as X, we have

$$ds^2=g_{ij}dx^idx^j=\rho(dx^2+dy^2+dz^2)+\psi(xdx+ydy+zdz)^2$$
$$+2\sigma(xdx+ydy+zdz)dt+\phi dt^2, \tag{7.2}$$

where ρ,ψ,σ and ϕ are any functions of r and t, and this is the well-known formula for spherically symmetric space-time. Next by using T_a and U, we know that these functions must be constant. Finally using [a], we have

$$ds^2=\rho(dx^2+dy^2+dz^2-(1/a)dt^2), \quad (\rho=\text{const.}), \tag{7.3}$$

as the general solution, which defines a Minkowski space-time.

On the other hand, in case of [b] and [c], we can easily show that there exists no g_{ij} satisfying (7.1). Therefore if we take a four dimensional space-time and assume the form-invariancy of its metric under the fundamental transformation group $\mathfrak{G}$ of our E.O. of the first kind, we have only to consider the case of [a] for which the desired space-time is given by (7.3).

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* Universal time can exist only in τ-measure in Milne's theory.

§ 8. Equivalent observers of the second kind

In this section we shall treat the E.O. of the second kind stated in § 4, i.e. those defined by the postulates (P. I), (P. II) and (P. IV) in § 4 and

(P. III′) *The group of frame-transformations* $\mathfrak{G}'_0$ *is given by the rotations* (4·2), *and this* $\mathfrak{G}'_0$ *forms a continuous group* $\mathfrak{G}'$ *together with the transformations given by* (4·1).

From the standpoint of the group $\mathfrak{G}'$, therefore, E.O. of this kind have not, in general, the properties of spatial and temporal homogeneities though they have spatial isotropy.

If we make similar considerations as in § 5 and § 6 with respect to transformations between E.O. of the second kind, we have (6.6) as the general solution of the equations obtained from (R_a,P_b). Then substituting this into the equations obtained from (P_a,P_b), and rewriting anew some suitable linear combinations (with constant coefficients) of P_a and R_b as P_a, we obtain the following theorem:

Theorem 2. *The most general transformation between two E.O. of the second kind is given by the following one provided we rotate* S_M *and* $S_{M'}$ *so that* MM' *coincides with x-axes of both* S_M *and* $S_{M'}$:

$$P_1=(x^2\rho+\tau)\partial_x+xy\rho\partial_y+xz\rho\partial_z+x\sigma\partial_t, \tag{8.1}$$

where ρ,τ *and* σ *are arbitrary functions of* r *and* t *satisfying*

$$\rho\tau-\{(\rho r^2+\tau)/r\}\tau'-\sigma\dot{\tau}=a, \tag{8.2}$$

$$(\dot{\tau})_{r=0}\neq 0, \quad \tau'=\partial\tau/\partial r, \quad (a \text{ is any const.}), \tag{8.3}$$

and for (8·1), *it holds that*

$$(P_a,P_b)=a\epsilon^{abc}R_c, \quad (R_a,P_b)=\epsilon^{abc}P_c. \tag{8.4}$$

If we put further assumptions on P_1, we have some interesting results as follows:

(i) If we assume $y'=y$ and $z'=z$ i.e. $\beta=\gamma=0$, we have

$$P_1=\tau\partial_x+x\sigma\partial_t \text{ with } \tau\tau'/r+\sigma\dot{\tau}+a=0, \quad (\dot{\tau})\neq 0. \tag{8.5}$$

(i_a) If we put $\tau=t$ in (8.5), P_1 becomes a transformation of the same form as Lorentz one.

(i_b) Next, if we put $\tau=(pe^{kt}+qe^{-kt})\sqrt{(1-k^2r^2)}$, $\sigma=k(pe^{kt}-qe^{-kt})/\sqrt{(1-k^2r^2)}$ and $a=4k^2pq$ where k,p and q are arbitrary constants, (8.5) is satisfied and we have

$$P_1=(pe^{kt}+qe^{-kt})\sqrt{(1-k^2r^2)}\partial_x+\{kx(pe^{kt}-qe^{-kt})\partial_t\}/\sqrt{(1-k^2r^2)}, \tag{8.6}$$

which was obtained by Sibata in his theory concerning the observation in cosmology in terms of wave geometry.[5] In his paper it is made clear that M' moves away from M with velocity proportional to their relative distance, and various properties of this transformation are also clarified.

(ii) If we assume that α,β,γ and δ are functions of x and t, we have

$$P_1=\tau(t)\partial_x-\{ax/(d\tau/dt)\}\partial_t, \tag{8.7}$$

properties of which will be clarified later using its finite form.

(iii) When $\tau=-(r^2+t^2)$, $\rho=2$, $\sigma=2t$ and $a=0$, we have

$$P_1=(x^2-y^2-z^2-t^2)\partial_x+2xy\partial_y+2xz\partial_z+2xt\partial_t. \tag{8.8}$$

This transformation was obtained by Page in his "New relativity" under the assumption that relative motion between observers is of constant acceleration (in his sense).[6]

(iv) Putting $\tau=e^{-kt}-k^2r^2$, $\rho=2k^2$, $\sigma=-2k$ and $a=0$ where k is a constant, we have

$$P_1=\{e^{-2kt}-k^2(r^2-2x^2)\}\partial_x+2k^2xy\partial_y+2k^2xz\partial_z-2kx\partial_t, \tag{8.9}$$

which gives a motion of de Sitter space-time in some coordinate system.[7] In the same way, by taking τ,ρ,σ and a suitably we can obtain

$$\frac{2kR}{\lambda}\left(e^{kt}-e^{-kt}\frac{r^2-2x^2}{4R^2}\right)\partial_x+\frac{kxy}{R\lambda}e^{-kt}\partial_y+\frac{kxz}{R\lambda}e^{-kt}\partial_z+\frac{x}{R(1+r^2/4R^2)}\partial_t, \tag{8.10}$$

and

$$-\frac{R}{t}\left(1+\frac{r^2-2x^2}{4R^2}\right)\partial_x+\frac{xy}{2Rt}\partial_y+\frac{xz}{2Rt}\partial_z-\frac{x}{R(1+r^2/4R^2)}\partial_t, \tag{8.11}$$

where $\lambda\equiv e^{kt}+e^{-kt}$. These are motions of de Sitter and Minkowski space-time in some coordinate systems respectively. Properties of these transformations were studied by one of the present writers.[7] An example of the transformation which satisfies (8.1) and (8.2) but does not satisfy (8.3) is given by

$$\left(1-\frac{r^2-2x^2}{4R^2}\right)\partial_x+\frac{xy}{2R^2}\partial_y+\frac{xz}{2R^2}\partial_z, \tag{8.12}$$

which gives a motion in the space-time of relativistic cosmology[7].

Next, we shall deduce the finite form for P_1 given in theorem 3. To do this we have only to solve

$$\begin{aligned}&\frac{dx'}{du}=x'^2\rho(r',t')+\tau(r',t'), \qquad \frac{dy'}{du}=x'y'\rho(r',t'),\\ &\frac{dz'}{du}=x'z'\rho(r',t'), \quad \frac{dt'}{du}=x'\sigma(r',t'),\end{aligned} \tag{8.13}$$

where u is the parameter of the transformation and

$$\begin{aligned}\rho(r',t')\tau(r',t')-[\{\rho(r',t')r'^2+\tau(r',t')\}/r'](\partial\tau(r',t')/\partial r')\\ -\sigma(r',t')(\partial\tau(r',t')/\partial t')=a\end{aligned} \tag{8.14}$$

under the condition that $x'=x$, $y'=y$, $z'=z$ and $t'=t$ for $u=0$. From (8.14), we have

$$\frac{y'}{y}=\frac{z'}{z}, \quad \frac{ax'^2+\tau^2(r',t')}{ax^2+\tau^2(r,t)}=\frac{y'^2}{y^2}, \quad \frac{r'dr'}{dt'}=\frac{r'^2\rho(r',t')+\tau(r',t')}{\sigma(r',t')}. \tag{8.15}$$

Hence expressing x', y' and z' as functions of t', substituting this into the last of (8.13) and integrating it, we can obtain the desired finite form of P_1. Though the calculations are complicated in general, we can obtain the results easily in some special cases. For

instance, the finite form of (ii) is given by

$$x'=\frac{x-V\tau(t)}{\sqrt{(1+aV^2)}},\ y'=y,\ z'=z,\ \tau(t')=\frac{\tau(t)+aVx}{\sqrt{(1+aV^2)}}, \tag{8.16}$$

where V is the parameter suitably chosen. In this transformation M' moves with arbitrary acceleration relative to M by virtue of the term $\tau(t)$. Hence by making use of this transformation we may construct a relativity of relative motion with arbitrary acceleration. If we regraduate time-frame by $\tau(t)=T$ and use T in place of t, (8.16) is reduced to the transformation of Lorentz type. We may regard this regraduation of time as a frame-transformation, but it is not contained in $\mathfrak{G}_0'$. Thus the meaning of the transformation (8.16) is different from that of Lorentz transformation.

We can make considerations similar to those in § 7 with respect to the E.O. of the second kind.

§ 9. Conclusion

As a result of our investigation it is shown that there exist various kinds of E.O. and the main problems concerning E.O. can be classified into the following three :

(1) How to define various kinds of E.O.,

(2) How to find the forms or properties of the coordinate transformations between E.O., and

(3) The problems concerning the physical laws represented by the invariant relations between E.O.

In this paper we have treated (1) and (2) mainly, and concerning (3) we have paid only a little attention.

Lastly we have to mention that the problems concerning the " observation " and the " structure of the physical space and time " are interwoven with the problem of E.O. But, as a first stage of investigation, we have only dealt with the problem of E.O. which can be discussed separately from the other two.

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References

1) E. A. Milne, *Kinematic Relativity*, Oxford, 1948.
2) H. P. Robertson, Rev. Mod. Phys. 5 (1933), 62.
3) See also T. Sibata, Journ. Sci. Hiroshima Univ. 16 (1952). (in press).
4) W. Pauli, *Relativitätstheorie*, Leipzig, 1921, p. 556.
5) T. Sibata, Journ. Sci. Hiroshima Univ. 11 (1941), 21.
6) L. Page, Phys. Rev. 49 (1936), 254.
7) H. Takeno, Journ. Sci. Hiroshima Univ. 11 (1942), 201.

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Temperature Effect on the Paramagnetic Resonance in Crystals

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Temperature effect through Boltzmann distribution on the position and the shape of paramagnetic resonance lines is studied on the assumption that the lattice structure is rigid. General formulae for the moments of any order are derived in the form of traces which can be interpreted physically as temperature averages of the quantities represented by the relevant operators. The explicit expressions for the zero-th, the first and the second moments are given on the basis of the one-ion approximation for the density matrix involved in the temperature average. As examples, applications of the formulae to the case of electronic-paramagnetic resonance in the system of equivalent free ions and to that of nuclear-paramagnetic resonance in electronic-paramagnetic crystals are discussed.

§ 1. Introduction

The variation of temperature produces many effects on the paramagnetic resonance absorption. There is good reason to believe that such a rather large change of the small crystalline splitting as is observed between room and helium temperatures in nickel fluosilicate crystal[1], is due to the thermal expansion and deformation of the crystal structure. The thermal motion of the magnetic atoms in crystals, especially through magnetic interactions, changes the shape of the absorption lines. This effect is observed in the nuclear paramagnetic resonance and utilized for the study of phase changes of crystals[2]. Furthermore, when the spin-lattice relaxation phenomena have appreciable contributions to the broadening of resonance line, it is expected that the absorption line width changes conspicuously with temperature[3]. Apart from the effects mentioned above, however, the temperature has effects on the magnetic resonance lines through the Boltzmann factors involved in the expression of absorption intensity, even when we are allowed to assume that the lattice structure is rigid. The last effect in particular will be investigated here in detail. Our method of attack is to calculate the moments of the line shape function. The essential advantage of this method is that it enables us to write the moments in the form of traces and these in turn can be calculated by using the one-atom wave functions. Waller[4] used already in 1932 this method in deriving the expression for the mean square frequency of spin absorption in the absence of any external field. Then in

order to dispose of the problem in the presence of initial splittings and external magnetic field, the idea of *semi-diagonal* and *non-diagonal* part of the hamiltonian was introduced by Broer[5] and developed in greater detail by Van Vleck[6] and the followers[7][8].

In Van Vleck's classical paper[6] on the dipolar broadening the last mentioned effects of temperature were neglected ; his treatment will be seen later as corresponding to the limiting case of very high temperature. The same effect has been considered by Pryce and Stevens[7] briefly. Their procedure is to expand the Boltzmann factor in powers of 1/kT. Then the moments can be written as the sum of the traces. They have given, however, the explicit expression only for the area in general form, the reduction of which to more convenient form for applications has not been performed. Also they have given only sketches of their procedure. Our treatment of Boltzmann factor is somewhat different from theirs as will be seen below.

General expressions for the moments of any order are obtained in the form of diagonal sums or traces of some operators which can be interpreted as the temperature averages of the operarors. Then, making use of an approximate form of the density matrix we derived more convenient expressions for the zeroth, the first and the second moments.

These general formulae are applied to two special cases : firstly, to the case of electronic-paramagnetic resonance in the system of free ions, *i.e.*, ions with completely degenerate spin multiplet, and secondly to that of nuclear-paramagnetic resonance in electronic-paramagnetic crystals. The effects investigated in the first case are very small at high temperatures and expected to become appreciable only in low temperature region. However, the experimental evidences for the effect are not yet available. As for the second case, the appearance of many lines in the proton resonance at helium temperatures in copper sulphate single crystal found by Bloembergen[9], is a typical example of the resonance line shifts, which can be treated rigorously by our present formulae.

§ 2. General description of the structure of energy levels

As was stated in the introduction, we assume the crystal to be rigid. The general form of the hamiltonian $\mathfrak{H}$ for the system of spins in the crystal under the influence of constant magnetic field H can be written as

$$\mathfrak{H}=\sum_i W_i+\sum_{i<j}\sum T_{ij}\,, \tag{1}$$

where W_i is the energy operator for the isolated i-th spin including the Zeeman energy, which we may term as *one-ion energy*, and T_{ij} denotes the spin-spin interaction between the i-th and j-th spin and is usually considered as being additively made up of exchange and magnetic dipolar interactions. The eigenvalues of the hamiltonian $\mathfrak{H}$ cluster usually about the centers which are obtained by summing up the energy eigenvalues of the individual spin without taking into account the interaction between themselves. *i.e.*, the eigenvalues of the one-ion energy term $\sum W_i$. As the first approximation, therefore, we shall retain only that part of the interaction which commutes with the one-ion energy term $\sum W_i$.

This we call with Broer[5] the *semi-diagonal* part of the interaction. This part can be diagonalized simultaneously with the one-ion energy term, so this selection corresponds to the first order perturbation process. The semi-diagonal part of T_{ij} can be constructed by some suitable projection operators[7,8].

It may be remarked in passing that the term "semi-diagonal" will be used with favour to indicate that part of the operator concerned which commutes with the one-ion energy term $\sum' W_i$ and will be denoted in the following by the bar on the operator. The eigen-states of the semidiagonal hamiltonian $\mathfrak{H}$ will be distinguished by the symbols n, n', ……, and their proper energies by E_n, $E_{n'}$,……, respectively.

Let, for example, all the paramagnetic ions be equivalent and the eigenvalues of the spin multiplet W_i be $\varepsilon_1,\varepsilon_2,\cdots\varepsilon_\omega$ in increasing order. We assume here, for the sake of simplicity, that they are non-degenerate. The eigenvalues of the one-ion energy term are, then, given by $\sum_1^\omega N_\alpha\varepsilon_\alpha$, where N_α indicates the number of spins which occupy the level ε_α, and they are $N!/\Pi N_\alpha!$-fold degenerate, respectively, where $N=\sum' N_\alpha$ is the total number of spins in the crystal. When the semi-diagonal interaction $\sum_{i<j}' \bar{T}_{ij}$ is introduced thereto, these $N!/\Pi N_\alpha!$ degenerate states couple only within themselves, and the energy levels split but cluster about the original position $\sum' N_\alpha\varepsilon_\alpha$. The non-diagonal interaction, *i.e.* $\sum_{i>j}(T_{ij}-\bar{T}_{ij})$, would have coupled these otherwise separated clusters, but only *slightly*, as assumed. The *resonance* line to be observed as the $\alpha\longleftrightarrow\beta$ transition consists of fine-structure components which combine each of the levels belonging to $(N_1, N_2,\ldots N_\alpha,\ldots N_\beta \ldots N_\omega)$ manifold and each of the levels belonging to $(N_1,N_2\ldots N_{\alpha-1}\ldots N_{\beta+1}\ldots N_\omega)$ manifold, where we may call these two clusters of levels neighbor clusters.

In case of the system of free spins with quatum number S, which will be treated in Section 4, Case I, eigenvalues of the one-ion energy W are equally spaced and moreover allowed transitions are those between neighbor clusters, so that all the transitions make equal jumps. This results in a strong resonance line with the frequency at $g\beta H/h$, which is usually called *Larmor line*. The improvement of the approximation, namely the inclusion of the non-diagonal part of the hamiltonian and the consideration of higher order perturbations, would afford subsidiary absorption lines, *i.e.*, the broadened weak lines with frequency centers at $0, 2g\beta H/h$, $3g\beta H/h$. (See Broer[5] and Van Vleck.[6])

§ 3. General Formulae for the Moments

When the paramagnetic crystal is placed in a weak oscillating magnetic field, it will make transitions between its eigen-states. This is caused by the parturbation energy $-$(Magnetic moment)$\cdot$(oscillating field). We are treating here the field classically and therefore neglect the spontaneous emission processes, which simplification is justifiable in the current *micro-wave* experiments. The probability for the single transition $n\rightarrow n'$ per unit time when the working field is spectrally continuous is given by

$$\frac{2\pi}{\hbar^2}|(n|\hat{M}|n')|^2 u_\nu,$$

where $\hat{M}$ is the operating component of the magnetic moment vector, its circumflex means that it has been freed from all the matrix components that are irrelative to the one-ion energy transition concerned, $\hat{M}$ being assumed to be a sum of the one-ion operator $\hat{M}_i$: $\hat{M}=\sum_i \hat{M}_i$, and $u_\nu d\nu$ is the energy in the high frequency field per unit volume in the frequency region $d\nu$ about $\nu=|E_{n'}-E_n|/h$. According to (1), the probability for the transition $n \rightarrow n'$ is equal to that for the inverse transition $n' \rightarrow n$. The non-vanishing absorption results, therefore, only from the higher population of the lower level. To formulate this situation quantitatively, we first define the absorption coefficient $A_{sec}(\nu)$: the amount of energy absorbed by the crystal per second in the frequency interval between ν and $\nu+d\nu$ should be $A_{sec}(\nu)\, u_\nu d\nu$. Then taking account of the Boltzmann distribution at temperature T, we easily obtain the expression for $A_{sec}\, d\nu$:

$$A_{sec}\, d\nu = h\nu Z^{-1} \sum_n (\exp(-E_n/kT) - \exp(-E_{n'}/kT)) \sum_{n'}^{+\Delta} (2\pi/\hbar^2) |(n|\hat{M}|n')|^2, \quad (2)$$

where the second summation $\sum_{n'}^{+\Delta}$ should be taken by definition over only those of n' which are consistent with the condition $h\nu \leq E_{n'} - E_n \leq h(\nu + d\nu)$, and Z is the partition function of the crystal and can be expressed in the form of trace:

$$Z = \sum_n \exp(-E_n/kT) = Tr(\exp(-\mathfrak{H}/kT). \quad (3)$$

We shall here investigate the functional form of the more frequently used quantity $\chi''(\nu)$, the imaginary part of the high frequency magnetic susceptibility, which is related to the above defined absorption coefficient A_{sec} by

$$A_{sec} = 8\pi^2 \nu \chi''. \quad (4)$$

Then we have instead of (2),

$$\chi'' d\nu = \frac{\pi}{h} Z^{-1} \sum_n (\exp(-E_n/kT) - \exp(-E_{n'}/kT)) \sum_{n'}^{+\Delta} |(n|\hat{M}|n')|^2. \quad (2')$$

If we could solve the eigenvalue problem of $\mathfrak{H}$ completely, we could have a full knowledge of the functional form of $\chi''(\nu)$ directly from the formula (2'). However, since the solution of this problem is out of the question, we are forced to turn to calculation of the moments of χ'' which are really obtainable in the form of diagonal sums of certain tractable operators.

The *zero-th moment*, which is sometimes called the *area*, is by definition

$$\int_0^\infty \chi''(\nu) d\nu = \frac{\pi}{h} Z^{-1} \sum_n \sum_{n'}^{+} (\exp(-E_n/kT) - (\exp(-E_{n'}/kT)) |(n|\hat{M}|n')|^2, \quad (5)$$

where the second summation $\sum'^{+}$ is to be taken over n''s which satisfy the condition $E_{n'} > E_n$. To avoid this restriction upon the summation over n', we introduce the operators $\hat{M}_+$ and $\hat{M}_-$ which are defined on the strength of $\mathfrak{H}$-representation as follows:

$$(n|\hat{M}_+|n') = \begin{cases} (n|\hat{M}|n'), & \text{for } E_{n'} < E_n, \\ 0, & \text{otherwise;} \end{cases} \quad (6a)$$

and

$$(n|\hat{M}_-|n') = \begin{cases} (n|\hat{M}|n'), & \text{for } E_{n'} > E_n, \\ 0 & \text{, otherwise.;} \end{cases} \tag{6b}$$

so that

$$\hat{M} = \hat{M}_+ + \hat{M}_- . \tag{6c}$$

These operators enable us to transform the expression (5) in a trace form:

$$\int_0^\infty \chi'' d\nu = \frac{\pi}{h} Z^{-1} \sum_n \sum_{n'} \left(\exp\left(\frac{-E_n}{kT}\right)(n|\hat{M}_-|n')(n'|\hat{M}_+|n)\right.$$

$$\left. -\exp\left(\frac{-E_{n'}}{kT}\right)(n'|\hat{M}_+|n)(n|\hat{M}_-|n')\right) = \frac{\pi}{h} Z^{-1} Tr(\exp(-\mathfrak{H}/kT)[\hat{M}_-, \hat{M}_+]), \tag{7}$$

where and hereafter the square bracket means the commutator of the two operators involved:

$$[A, B] = AB - BA.$$

The last expression, however, means physically the statistical average of the operator $(\pi/h) \cdot [\hat{M}_-, \hat{M}_+]$ at temperature T, which we shall indicate with the symbol $< >_T$:

$$\int_0^\infty \chi'' d\nu = < \frac{\pi}{h} [\hat{M}_-, \hat{M}_+] >_T . \tag{7'}$$

The advantage of such a trace form is that the invariance of the diagonal sum makes it unnecessary to know the stationary states n.... Instead the trace can be computed in an arbitrary system of quantization, most conveniently one in which H_i's are individually diagonalized (one-ion observable representation). The usefulness of the formulae (7) may, therefore, be decided whether it is possible to define the operators $\hat{M}_+$ and $\hat{M}_-$ in terms of the one-ion observable representation. According to the level scheme explained in Section 2, the energy E_n of an eigen-state of $\mathfrak{H}$ is the sum of an one-ion energy sum and a semi-diagonal intetaction energy term. In case of the resonance absorption $\hat{M}$ should have matrix elements only between such states as have the energy difference in the one-ion energy sum. Since the interaction energy is smaller than this difference, as assumed, the superiority in the one-ion energy sum necessarily entails the superiority in the semi-diagonal energy, when we are comparing the semi-diagonal energies of states. Therefore it is quite practicable to construct the operators $\hat{M}_+$ and $\hat{M}_-$ on the basis of one-ion observable representation in case of the resonance absorption. For example, we take up again the system of equivalent paramagnetic ions. For this system, the one-ion energy can be written as $\sum_\alpha N_\alpha \varepsilon_\alpha$. When we observe the resonance absorption corresponding to the $\alpha \longleftrightarrow \beta$ transition, $\hat{M}$ should have matrix elements only between states which have energy difference $\varepsilon_\alpha - \varepsilon_\beta$ in the one-ion energy sum, where we assumed $\varepsilon_\alpha > \varepsilon_\beta$. When we introduce the projection operator $P_{\alpha i}$ for the states, in which the i-th ion must have ε_α as the one-ion energy, and the operators $\hat{M}_{+i}$ and $\hat{M}_{-i}$, which are defined by $P_{\alpha i} M_i P_{\beta i}$ and $P_{\beta i} M_i P_{\alpha i}$ respectively, we can define $\hat{M}_+$ and $\hat{M}_-$ by $\sum \hat{M}_{+i}$ and $\sum \hat{M}_{-i}$ respectively. In contrast to the above case, these

operators are unmanageable with the one-ion representation in case of those non-resonant or "zero-frequency" lines (the spin-absorption) which are experimented extensively by Dutch school[10].

The *first moment* can be derived straightforwardly. In this case it is quite unnecessary to use $\hat{M}_+$ or $\hat{M}_-$. From Eq. (2),

$$h\int_0^\infty \nu\chi'' d\nu = \frac{\pi}{h} Z^{-1} \sum_n \sum_{n'}{}^{+} (E_{n'}-E_n)\,(\exp(-E_n/kT)-\exp(-E_{n'}/kT)) \times \times |(n|\hat{M}|n')|^2$$

$$= \frac{\pi}{2h} Z^{-1} \sum_n \sum_{n'} (E_{n'}-E_n)\,(\exp(-E_n/kT)-\exp(-E_{n'}/kT)) \times \times |(n|\hat{M}|n')|^2$$

$$= \frac{\pi}{2h} Z^{-1}\, Tr(\exp(-\bar{\mathfrak{H}}/kT)[\hat{M},[\bar{\mathfrak{H}},\hat{M}]])$$

$$= \frac{\pi}{2h} <[\hat{M},[\bar{\mathfrak{H}},\hat{M}]]>_T \qquad (8)$$

It should be specially remarked here that Eq. (8) is practicable also in the "zero-frequency" case.

In order to derive the *second moment*, it is again necessary to use $\hat{M}_+$ and $\hat{M}_-$:

$$h^2\int_0^\infty \nu^2\chi'' d\nu = \frac{\pi}{h} Z^{-1} \sum_n \sum_{n'}{}^{+} (E_n-E_{n'})^2 (\exp(-\frac{E_n}{kT})-\exp(-\frac{E_{n'}}{kT}))\,|(n|\hat{M}|n')|^2$$

$$= \frac{\pi}{h} Z^{-1}\, Tr(\exp(-\bar{\mathfrak{H}}/kT)[[\hat{M}_-,\bar{\mathfrak{H}}],[\bar{\mathfrak{H}},\hat{M}_+]])$$

$$= \frac{\pi}{h} \langle[[\hat{M}_-,\bar{\mathfrak{H}}],[\bar{\mathfrak{H}},\hat{M}_+]]\rangle_T \qquad (9)$$

It may be possible to foresee how to generalize these formulae and how the $\hat{M}_+$ and $\hat{M}_-$ operators are to appear in the expressions for the moments of *even* order in contrast with those for the moments of *odd* order which involve only the $\hat{M}$ operator. The derived formulae can be written compactly as follows:

$$\int_0^\infty (h\nu)^{2l}\,\chi'' d\nu = \frac{\pi}{h} \langle[\{\hat{M}_-,\bar{\mathfrak{H}}\}^l,{}^l\{\bar{\mathfrak{H}},\hat{M}_+\}]\rangle_T \qquad (10a)$$

and

$$\int_0^\infty (h\nu)^{2l-1}\chi'' d\nu = \frac{\pi}{2h} \langle[\{\hat{M},\bar{\mathfrak{H}}\}^{l-1},{}^l\{\bar{\mathfrak{H}},\hat{M}\}]\rangle_T, \qquad (10b)$$

where the symbols $\{\ \}^l$ and ${}^l\{\ \}$ represent the iterated commutators of the following

types :

$$\{A,\bar{\mathfrak{H}}\}^l=[[\cdots[[A,\underset{1}{\bar{\mathfrak{H}}}],\underset{2}{\bar{\mathfrak{H}}}],\cdots],\underset{l}{\bar{\mathfrak{H}}}]$$

and

$${}^l\{\bar{\mathfrak{H}},A\}=[\underset{1}{\bar{\mathfrak{H}}},[\underset{2}{\bar{\mathfrak{H}}},[\cdots[\underset{l}{\bar{\mathfrak{H}}},A]\cdots]]]=(-1)^l\{A,\bar{\mathfrak{H}}\}^l,$$

the derivation of which are given in the Appendix. Similar remarks mentioned after Eqs. (7′) and (8) are also applicable here.

In conclusion some relations used below will be added. The mean frequency $<\nu>_{AV}$ which is defined as

$$<\nu>_{AV}=\int_0^\infty\int_0^\infty \nu\chi''d\nu\,\chi''d\nu\Big/\int_0^\infty\chi''d\nu,$$

is in general different from the original frequency ν_0, that is the absorption frequency when the interactions between spins were absent, a pure one-ion quantity. The deviation will be denoted as

$$<\Delta_0\nu>_{AV}=<\nu>_{AV}-\nu_0. \tag{11}$$

An idea of the line width can be given with the mean square deviation about the mean frequency $<\nu>_{AV}$:

$$<\Delta\nu^2>_{AV}=<\nu^2>_{AV}-<\nu>^2. \tag{12}$$

As a matter of course, the computation of higher moments may increase knowledge about the functional form of $\chi''(\nu)$, but it is usually formidable or even unpracticable.

§ 4. Approximation for the density matrix

In order to proceed further, we must make a certain approximation for the density matrix $\exp(-\bar{\mathfrak{H}}/kT)$. Since $\bar{\mathfrak{H}}=\sum_i W_i+\sum_{i<j}\bar{T}_{ij}$, we have as a first approximation for the relatively high temperatures

$$\exp(-\bar{\mathfrak{H}}/kT)=\Pi_i\rho_i,\quad \text{with}\ \rho_i=\exp(-W_i/kT), \tag{13}$$

where the interaction terms are neglected. This approximation becomes less accurate when the temperature lowers and it is completely inadequate below the curie temperature, where ferro- or antiferromagnetic state sets in.

The total magnetic moment $\hat{M}$ can be written as

$$\hat{M}=\sum_i\hat{M}_i=\sum_i(\hat{M}_{+i}+\hat{M}_{-i}). \tag{14}$$

Substituting Eqs. (1)(13) and (14) into Eqs. (7)(8) and (9), we can derive more convenient formulae for calculations. In doing so, we must observe that the operators without common suffices are commutable. We obtain after some elementary calculations

$$\int_0^\infty \chi'' d\nu = \frac{\pi}{h} \sum_j (Tr\ \rho_j)^{-1} Tr(\rho_j [\hat{M}_{-j}, \hat{M}_{+j}]), \tag{15}$$

$$h\int_0^\infty \nu\chi'' d\nu = \frac{\pi}{2h} \{ \sum_j (Tr\rho_j)^{-1} Tr(\rho_j [\hat{M}_j, [W_j, \hat{M}_j]]) +$$

$$+ \sum_j \sum_{k(\neq j)}' (Tr(\rho_j \rho_k))^{-1} Tr(\rho_j \rho_k [\hat{M}_j, [\bar{T}_{jk}, \hat{M}_j + \hat{M}_k]]),$$

$$h^2 \int_0^\infty \nu^2 \chi'' d\nu = \frac{\pi}{h} [\sum_j (Tr\ \rho_j)^{-1}\ Tr(\rho_j [[W_j, \hat{M}_{+j}], [W_j, \hat{M}_{-j}]]) +$$

$$+ \sum_j \sum_{k(\neq j)}' (Tr(\rho_j \rho_k))^{-1} Tr(\rho_j \rho_k \{ [[\bar{T}_{jk}, \hat{M}_{+j} + \hat{M}_{+k}], [W_j, \hat{M}_{-j}]] +$$

$$+ [[W_j, \hat{M}_{+j}], [\bar{T}_{jk}, \hat{M}_{-j} + \hat{M}_{-k}]] + \tfrac{1}{2} [[\bar{T}_{jk}, \hat{M}_{+j} + \hat{M}_{+k}],$$

$$[\bar{T}_{jk}, \hat{M}_{-j} + \hat{M}_{-k}]] \}) +$$

$$+ \sum_j \sum_{k(\neq j)}' \sum_{h(\neq j,k)}'' (Tr(\rho_j \rho_k \rho_h))^{-1} Tr(\rho_j \rho_k \rho_h [[\bar{T}_{jk}, \hat{M}_{+j} + \hat{M}_{+k}],$$

$$[\bar{T}_{jh}, \hat{M}_{-j} + \hat{M}_{-h}]])]. \tag{17}$$

Now we apply these formulae to two special cases.

Case I. Degenerate spin multiplet

Here we consider a paramagnetic crystal in which each paramagnetic ion is equivalent and has, as the lowest energy term, a degenerate spin multiplet. When the static field is along the z-direction, W_j can be written as

$$W_j = g\beta H S_{zj}, \tag{18}$$

where S_{zj} is the z-component of the spin vector of j-th ion, g is the Lande factor, β the Bohr magneton, and H is the intensity of magnetic field.

We also have if the oscillating field is along the x-direction,

$$\hat{M}_j = -g\beta S_{xj}, \tag{19a}$$

hence

$$\hat{M}_{\pm j} = -\frac{g\beta}{2} S_{\pm j} = -\frac{g\beta}{2} (S_{xj} \pm i\ S_{yj}), \tag{19b}$$

where we are considering the Larmor line, which is broadened about the Larmor precession frequency $\nu_0 = g\beta H/h$.

As was shown by Van Vleck[6], the semi-diagonal part of the interaction term between the j-th and the k-th spin can be written as

$$\bar{T}_{jk} = A_{jk} S_j \cdot S_k + B_{jk} S_{zj} \cdot S_{zk} \tag{20}$$

with

$$A_{jk} = \tilde{A}_{jk} + g^2\beta^2 r_{jk}^{-3} \left[\frac{3}{2} \gamma_{jk}^2 - \frac{1}{2} \right] \tag{21}$$

and

$$B_{jk}=-3g^2\beta^2 r_{jk}^{-3}\left[\frac{3}{2}\gamma_{jk}^2-\frac{1}{2}\right],$$

where $\tilde{A}_{jk}$ is the coefficient of the exchange interaction, r_{jk} is the distance between the j-th and the k-th spin and γ_{jk} is the direction cosine of r_{jk} relative to the z-axis.

Applying Eqs. (13), (14) and (15) to this case, we find that

area : $$\int_0^\infty \chi'' d\nu=\frac{-\pi}{2h}Ng^2\beta^2<S_{zi}>_T, \tag{22}$$

the first moment :

$$h\int_0^\infty \nu\chi'' d\nu=-\frac{\pi}{2h}Ng^2\beta^2<S_{zi}>_T\left[g\beta H+<S_{zi}>_T\sum_{k(\neq j)}{}'B_{jk}\right], \tag{23}$$

the second moment :

$$h^2\int_0^\infty \nu^2\chi'' d\nu=-\frac{\pi}{2h}Ng^2\beta^2<S_{zi}>_T\Big[(g\beta H+<S_{zi}>_T\sum_{k(\neq j)}{}'B_{jk})^2 + (<S_{zi}^2>_T-<S_{zi}>_T^2)\sum_{k(\neq j)}{}'B_{jk}^2\Big], \tag{24}$$

where N denotes the total number of spins.

Since $\nu_0=g\beta H/h$, we have from Eqs. (16), (17), (22), (23) and (24)

$$<\Delta_0\nu>_{AV}=\frac{1}{h}<S_{zi}>_T\sum_{k(\neq j)}{}'B_{jk}, \tag{25}$$

$$<\Delta\nu^2>_{AV}=\frac{1}{h^2}(<S_{zi}^2>_T-<S_{zi}>_T^2)\sum_{k(\neq j)}{}'B_{jk}^2. \tag{26}$$

We can, however, obtain $<S_{zi}>_T$ and $<S_{zi}^2>_T$ as functions of temperature explicitly, the forms of which are as follows :

$$<S_{zi}>_T=\sum_{M=-S}^{S}M\exp(-g\beta HM/kT)\Big/\sum_{M=-S}^{S}\exp(-g\beta HM/kT)=-SB_s(y) \tag{27}$$

and

$$<S_{zi}^2>_T=\sum_{M=-S}^{S}M^2\exp(-g\beta HM/kT)\Big/\sum_{M=-S}^{S}\exp(-g\beta HM/kT)=S^2\left(B_s^2(y)+\frac{d}{dy}B_s(y)\right) \tag{28}$$

with $$y=g\beta HS/kT,$$

where $B_s(y)$ is the Brillouin function and has the form :

$$B_s(y)=\frac{2S+1}{2S}\coth\left(\frac{2S+1}{2S}y\right)-\frac{1}{2S}\coth\frac{y}{2S}. \tag{29}$$

First we consider the displacement (25), this can be written as

$$<\Delta_0\nu>_{AV}=-\frac{3}{2}\frac{<M_z>_T}{N_1H}\nu_0\sum_k r_{ik}^{-3}(1-3\gamma_{ik}^2), \tag{30}$$

where $<M_z>_T$ is the z-component of the intensity of magnetization and N_1 is the number of spins per unit volume. The sum in Eq. (30) is dependent on the shape of the sample used in the experiment. When the sample is ellipsoidal in shape and is orientated with one of its principal axes along the static field, the classical demagnetization factor N_z can be used instead of the sum according to the relation[11]

$$N_z = N_1^{-1} \sum_k{}' r_{jk}^{-3}[1-3\gamma_{ik}^2] + (4\pi/3). \tag{31}$$

Then, Eq. (30) becomes

$$<\Delta_0\nu>_{AV} = \frac{3}{2}\nu_0\chi_z\left(\frac{4\pi}{3} - N_z\right), \tag{32}$$

where $\chi_z = <M_z>_T/H$ is the static magnetic susceptibility (per unit volume). In the temperature range of *normal* paramagnetism the following approximate formula holds,

$$<\Delta_0\nu>_{AV} = \frac{1}{2}N_1\nu_0\frac{g^2\beta^2S(S+1)}{kT}\left(\frac{4\pi}{3} - N_z\right). \tag{33}$$

Since except at low temperatures χ_z has usually only a very small value ($\sim 10^{-5}$), $<\Delta_0\nu>_{AV}$ is negligible at room temperatures.

The expression for the mean square deviation $<\Delta\nu^2>$ differs from that of Van Vleck in the factor $(<S_{zi}^2>_T - <S_{zi}>_T^2)$, which is replaced by $\frac{1}{3}S(S+1)$ in Van Vleck's expression. If the temperature is high and the field intensity is not so strong as to produce saturation effects, we can expand the factor $(<S_{zi}^2>_T - <S_{zi}>_T^2)$ in the inverse powers of kT, and we find

$$<S_{zi}^2>_T - <S_{zi}>_T^2 = \frac{1}{3}S(S+1) - \frac{1}{30}S(S+1)[2S(S+1)+1]\left(\frac{h\nu_0}{kT}\right)^2 + \cdots. \tag{34}$$

When we retain only the first term in the right hand, we obtain Van Vleck's result. The second and the higher terms in the Eq. (34) are negligible at room temperature, since in experiments ν_0 is usually about 10 kMC and consequently $h\nu_0/kT$ is only 10^{-3} at room temperature. At low temperatures the higher order terms may not be negligible.

At extremely low temperature, where our approximation for the density matrix becomes inadequate, the above expressions do not hold. We shall give some improved treatment for this case in a later paper.

For the nuclear magnetic resonance experiment in diamagnetic crystals, the above derived expressions can be adopted when we replace the spin S with the nuclear spin I, and $g\beta$ with $\gamma\hbar$, where γ is the gyromagnetic ratio characteristic of the nuclei under consideration. Then we find that χ_z involved in *Eq.*(32) is much smaller than that of electronic paramagnetism, so $<\Delta_0\nu>_{AV}$ is much more negligible. The second term in Eq. (34) becomes also much smaller, since in current nuclear resonance experiments $\nu_0 \sim 10$ *MC* and $h\nu_0/kT \sim 10^{-6}$ at room temperatures.

Case II. The Effect of Electronic-Paramagnetic Ions on the Nuclear Resonance

As in the case of the proton-resonance in paramagnetic crystals, the nuclear resonance lines must be disturbed greatly by the presence of paramagnetic ions in the crystal.

In this case we have two magnetic ingredients, namely one is nucleus with magnetic moment $\mu=\gamma\hbar I$, another is paramagnetic ion with magnetic moment $-g_i\beta S$, but the treatment in this section can be applied *mutatis mutandis*. We consider the Larmor resonance, so we have

$$\mathcal{W}_\nu=-\gamma\hbar H I_{z\nu} \tag{35}$$

and

$$\hat{M}_\nu=\gamma\hbar I_{x\nu}, \tag{36}$$

where we use Greek suffices for numbering nuclei, which have gyromagnetic ratio γ and spin I.

If we consider only the effect of paramagnetic ions on the line and disregard the interactions between the same type spins, we can write as the relevant interaction term between the ν-th nucleus and the i-th paramagnetic ion,

$$\begin{aligned}\bar{T}_{i\nu}&=(A_{i\nu}+B_{i\nu})S_{zi}\cdot I_{z\nu}\\&=\frac{g\beta\cdot\gamma\hbar}{r_{i\nu}^3}(3\gamma_{i\nu}^2-1)S_{zi}\cdot I_{z\nu}.\end{aligned} \tag{37}$$

The assignment of $M_{\pm\nu}$ to $\gamma\hbar I_{\pm\nu}$ is different according to the sign of the gyromagnetic ratio γ. For $\gamma>0$, we have

$$\hat{M}_{+\nu}=\frac{1}{2}\gamma\hbar I_{-\nu}=\frac{1}{2}\gamma\hbar(I_{x\nu}-iI_{y\nu})$$

and (38)

$$\hat{M}_{-\nu}=\frac{1}{2}\gamma\hbar I_{+\nu}=\frac{1}{2}\gamma\hbar(I_{x\nu}+iI_{y\nu}),$$

but for $\gamma<0$,

$$\hat{M}_{+\nu}=\frac{1}{2}\gamma\hbar I_{+\nu}$$

and (39)

$$\hat{M}_{-\nu}=\frac{1}{2}\gamma\hbar I_{-\nu}.$$

We assume $\gamma>0$ in the following calculations.

From Eqs. (13), (14) and (15), we find the following results:

the area: $\displaystyle\int_0^\infty\chi''d\nu=\frac{\pi}{h}\sum_\nu(Tr\,\rho_\nu)^{-1}\,Tr(\rho_\nu[\hat{M}_{-\nu},\hat{M}_{+\nu}])$

$$=\frac{\pi}{4h}N(\gamma\hbar)^2<[I_{+\nu},I_{-\nu}]>_T=\frac{\pi}{2h}N(\gamma\hbar)^2<I_{z\nu}>_T. \tag{40}$$

the first moment:

$$h\int_0^\infty \nu\chi''d\nu=\frac{\pi}{2h}\{\sum_\nu (Tr\,\rho_\nu)^{-1}Tr(\rho_\nu[\hat{M}_\nu,[W_\nu,\hat{M}_\nu]])+$$

$$+\sum_\nu\sum_j (Tr(\rho_\nu\rho_j))^{-1}\,Tr(\rho_\nu\rho_j[\hat{M}_\nu,[\bar{T}_{\nu j},\hat{M}_\nu]])\}$$

$$=\frac{\pi}{2h}N(\gamma\hbar)^2<I_{z\nu}>_{\mathrm{av}}\gamma\hbar(H+\sum_j g\beta<S_{zj}>_T r_{j\nu}^{-3}[1-3\gamma_{j\nu}^2]), \qquad (41)$$

where j is used for numbering the paramagnetic ion. The second term in the parenthesis may be considered as representing the effective internal field produced by the paramagnetic ions at the ν-th nucleus.

Then we have

$$<\Delta_0\nu>_{AV}=h^{-1}\sum_j\gamma\hbar g\beta<S_{zj}>_T r_{j\nu}^{-3}(1-3\gamma_{j\nu}^2) \qquad (42)$$

as the deviation of the mean frequencies from the original frequency $\gamma\hbar/h$. The second moment and the mean square deviation frequency can be calculated easily. We find

$$<\Delta\nu^2>_{AV}=h^{-2}(\gamma\hbar g\beta)^2\sum_j(<S_{zj}^2>_T-<S_{zj}>_T^2)r_{j\nu}^{-6}(1-3\gamma_{j\nu}^2)^2 \qquad (43)$$

as the contribution of the paramagnetic ions to the mean square deviation of nuclear magnetic resonance line.

In the temperature range of the *normal* paramagnetism, we have from Eqs. (34) and (43)

$$<\Delta_0\nu>_{AV}=h^{-1}\sum_j\gamma\hbar g\beta[S(S+1)/(3kT)]r_{j\nu}^{-3}(1-3\gamma_{j\nu}^2),$$

and (44)

$$<\Delta\nu^2>_{AV}=h^{-2}(\gamma\hbar g\beta)^2\frac{1}{3}S(S+1)\sum_j r_{j\nu}^{-6}(1-3\gamma_{j\nu}^2)^2.$$

When the g-values of paramagnetic ions are anisotropic, we must introduce the g-tensors and replace $g\beta\,S_{jz}$ with $\beta(g_j\cdot S_j)_z$ in the above formulae.

The temperature shifts of the above type is first observed by Bloembergen[9], who measured the proton resonance in the single crystal of copper sulphate from room temperatures, to liquid helium temperatures. He found many lines at liquid helium temperatures. This corresponds to the fact that in a unit cell of this crystal there are five inequivalent water molecules relative to the two paramagnetic ions, which produce different internal fields at the proton-pairs of water molecules. Poulis[12] found the similar phenomena in the single crystal of $CuCl_2\cdot 2H_2O$, which contain two inequivalent water molecules.

The formula (42) cannot be applied to these cases without alterations, since in these crystals the protons in a water molecule are interacting so strongly that we must take the hamiltonian for a two proton system as W_i. In a classical picture, the magnetic fields at the positions of two protons in a water molecule are not equal in general, since the internal fields produced by the cupric ions are different at these positions. The internal field at the ν-th proton is given by the expression

$$H_{\nu z}^{int}=\sum_i g\beta <S_{zi}>_T r_{i\nu}^{-3}(1-3\gamma_{i\nu}^2). \tag{45}$$

In Bloembergen's and Poulis' treatments the idea of internal field is introduced from the beginning without any justification from the first principle. We showed a more rigorous procedure above, and derived the internal field straightforwardly. The results will be, however, identical with theirs, therefore we don't reproduce them here.

§ 5. Discussion and conclusion

The effects of the Boltzmann factors involved in the expressions we derived are usually small at high temperatures. But at low temperatures they become appreciable. In case II in section 4, $<\Delta_0\nu>_{AV}$ is particularly large at liquid helium temperatures, because the ratio $\gamma\hbar/g\beta$ is as large as the ratio of the mass of proton and that of electron.

In our treatment, the most serious errors may come from the approximation of the density matrix made in section 4. The improvement of this approximation is one of the difficult but important problems in the statistical mechanics. Our approximation is the most crude one, since we have neglected interaction terms wholly. If we retain the interaction terms in the density matrix, we must find some devices in calculating the traces in our formulae. The expansion of the interaction terms into a power series of $1/kT$ will be a useful device, which was used by Van Vleck[11] in calculating the thermal and magnetic properties of paramagnetic substances. Another expansion was introduced by Kubo[13], who made use of another parameter instead of $1/kT$. The calculation of the moments by utilizing these expansions will be very interesting. We intend to perform it.

Another important problem related closely to ours is the spin-absorption[14]. The shape factor in this case is defined by

$$f(\nu)=\nu^{-1}\chi''(\nu),$$

so the area and first moment of this paper correspond to the first and the second moment of $f(\nu)$. As we derived in Section 3, the first moment of $f(\nu)$ will be expressed in a trace form only by introducing operators $\hat{M}_+$ and $\hat{M}_-$. In case of the spin-absorption (zero-frequency line), these operators are unmanageable in the one-ion observable representation we used in this paper. In contrast to it, the area and the second moment of $f(\nu)$ may be calculated by using only $\hat{M}_z$ which is manageable.

As to the application of our formulae to special cases, the presence of small initial splittings produced by the crystalline fields will complicate the problem to some extent. But the introduction of suitable projection operators will make the calculation practicable. (See for instance I.K.U.[8]).

We are desirous of measurements of the paramagnetic resonance at extremely low temperatures, including the determination of the line shape.

In conclusion, the authors wish to express their gratitude to Professor M. Kotani for his encouragements, and they also appreciate discussions of Professor E. Ishiguro.

Appendix

Derivation of Eq. (10*a*)

From Eq. (2′) we have

$$\int_0^\infty (h\nu)^{2l}\chi''d\nu=\frac{\pi}{h}Z^{-1}\sum_n\sum_{n'}{}'(E_{n'}-E_n)^{2l}(\exp(-E_n/kT)-\exp(-E_{n'}/kT))\times$$

$$\times|(n|\hat{M}|n')|^2=\frac{\pi}{h}Z^{-1}\sum_n\sum_{n'}\sum_{m=0}^{2l}\binom{2l}{m}(-1)^m E_{n'}^{2l-m}E_n^m(\exp(-E_n/kT)-\exp(-E_{n'}/kT))\times$$

$$\times(n|\hat{M}_-|n')(n'|\hat{M}_+|n)=\frac{\pi}{h}\sum_m(-1)^m\binom{2l}{m}Z^{-1}Tr(\exp(-\bar{\mathfrak{H}}/kT)(\bar{\mathfrak{H}}^m\hat{M}_-\bar{\mathfrak{H}}^{2l-m}\hat{M}_+-$$

$$-\bar{\mathfrak{H}}^{2l-m}\hat{M}_+\bar{\mathfrak{H}}^m\hat{M}_-))=\frac{\pi}{h}\sum_m(-1)^m\binom{2l}{m}\langle[\bar{\mathfrak{H}}^m\hat{M}_-,\bar{\mathfrak{H}}^{2l-m}\hat{M}_+]\rangle_T. \qquad \text{(A, 1)}$$

Now we can show easily by the mathematical induction

$$\{\hat{M}_-,\bar{\mathfrak{H}}\}^l=\sum_{n=0}^{l}(-1)^n\binom{l}{n}\bar{\mathfrak{H}}^n\hat{M}_-\bar{\mathfrak{H}}^{l-n},$$

and

$$^l\{\bar{\mathfrak{H}},\hat{M}_+\}=(-1)^l\{\hat{M}_+,\bar{\mathfrak{H}}\}^l=\sum_{k=0}^{l}(-1)^{l+k}\binom{l}{k}\bar{\mathfrak{H}}^k\hat{M}_+\bar{\mathfrak{H}}^{l-k}$$

$$=\sum_{k=0}^{l}(-1)^k\binom{l}{l-k}\bar{\mathfrak{H}}^{l-k}\hat{M}_+\bar{\mathfrak{H}}^k.$$

Then

$$[\{\hat{M}_-,\bar{\mathfrak{H}}\}^l\,{}^l\{\bar{\mathfrak{H}},\hat{M}_+\}]=\sum_{n=0}^{l}\sum_{k=0}^{l}(-1)^{n+k}\binom{l}{n}\binom{l}{n-k}[\bar{\mathfrak{H}}^n\hat{M}_-\bar{\mathfrak{H}}^{l-n},\bar{\mathfrak{H}}^{l-k}\hat{M}_+\bar{\mathfrak{H}}^k].$$

Hence

$$<[\{\hat{M}_-,\bar{\mathfrak{H}}\}^l\,{}^l\{\bar{\mathfrak{H}},\hat{M}_+\}]>_T=\sum_{n=0}^{l}\sum_{k=0}^{l}(-1)^{n+k}\binom{l}{n}\binom{l}{l-k}<[\bar{\mathfrak{H}}^{n+k}\hat{M}_-,\bar{\mathfrak{H}}^{2l-n-k}\hat{M}_+]>_T$$

$$=\sum_{m=0}^{2l}(-1)^m\Big[\sum_{n+k=m}\binom{l}{n}\binom{l}{l-k}\Big]<[\bar{\mathfrak{H}}^m\hat{M}_-,\bar{\mathfrak{H}}^{2l-m}\hat{M}_+]>_T$$

$$=\sum_{m=0}^{2l}(-1)^m\binom{2l}{m}<[\bar{\mathfrak{H}}^m\hat{M}_-,\bar{\mathfrak{H}}^{2l-m}\hat{M}_+]>_T, \qquad \text{(A,2)}$$

since $\sum_{n+k=m}\binom{l}{n}\binom{l}{l-k}=\binom{2l}{m}$, where the summation must be taken over all n's and k's consistent with the condition $n+k=m$.

Combining (A,1) and (A,2), we obtain the formula (10a).

Derivation of Eq. (10*b*)

From Eq.(2′) we can show similarly

$$\int_0^\infty (h\nu)^{2l-1}\chi''d\nu = \frac{\pi}{2l}\sum_{m=0}^{2l-1}(-1)^m\binom{2l-1}{m} <[\bar{\mathfrak{H}}^m\hat{M}, \bar{\mathfrak{H}}^{2l-1-m}\hat{M}]>_T \qquad \text{(B,1)}$$

And we have also

$$<[\{\hat{M},\bar{\mathfrak{H}}\}^{l-1}, {}^l\{\bar{\mathfrak{H}},\hat{M}\}]>_T = \sum_{m=0}^{2l-1}(-1)^m\binom{2l-1}{m} <[\bar{\mathfrak{H}}^m\hat{M}, \bar{\mathfrak{H}}^{2l-1-m}\hat{M}]>_T . \qquad \text{(B,2)}$$

Hence Eq. (10b) is verified.

References

1) R. P. Penrose and K.W.H. Stevens, Proc. Phys. Soc. **A63** (1950), 29.
2) H. S. Gutowsky and G.E. Pake, J. Chem. Phys. **18** (1950), 162, and other papers by various authors.
3) B. Bleaney and H.E.D. Scovil, Proc. Phys. Soc. **A64** (1951), 204. G. S. Bogle, A.H. Cooke and S. Whitley, Proc. Phys. Soc. **A64** (1951), 931.
4) I. Waller, ZS. f. Phys. **79** (1932), 380.
5) L. J. F. Broer, Physica **10** (1943), 801.
6) J. H. Van Vleck, Phys. Rev. **74** (1948), 1168.
7) M. H. L. Pryce and K. W. H. Stevens, Proc. Phys. Soc. **A 63** (1950), 36.
8) E. Ishiguro, K. Kambe and T. Usui, Physica **17** (1951), 310; Phys. Rev. **82** (1951), 680.
9) N. Bloembergen, Physica **16** (1950), 95.
10) C. J. Gorter, "*Paramagnetic Relaxation*" (Elsevier Publishing Co. Inc. 1947).
11) J. H. Van Vleck, J. Chem. Phys. **5** (1937), 320.
12) N. Poulis and G. E. G. Hardeman, Physica **18** (1952), 201, 315.
13) R. Kubo, J. Chem. Phys. **20** (1952), 770.
14) See Broer[5] and Gorter[10], especially Chap. IV, §3.

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On the Spherically Symmetric Space-Times in General Relativity

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Spherically symmetric space-times play important roles in general relativity. In this note a theory is developed concerning the problem of determining whether or not a space-time defined by a line element arbitrarily given in any coordinate system is spherically symmetric, using the concept of characteristic system introduced by the present author. Then, as an example, the theory is applied to the space-times of Weyl and Levi-Civita, of Gödel and of Silberstein.

§ 1. Introduction

A spherically symmetric space-time is a four dimensional Riemannian space whose line element is reducible to the form:

$$ds^2 = -A(r, t)dr^2 - B(r, t)(d\theta^2 + \sin^2\theta d\phi^2) + C(r, t)dt^2. \qquad (1\cdot1)$$

We shall denote this space-time by S_0. S_0 has played an important role in the general theory of relativity and we may rather say that the relativistic theory of cosmology has developed with the advance of the investigation concerning the spherically symmetric space-times.

For example, the space-time of Schwarzschild's exterior solution which provided the decisive experimental verification of general relativity (i.e. the famous three crucial tests) was obtained by solving the Einstein's field equation under the assumption of spherical symmetry. Moreover the space-time used in relativistic cosmology, in which the space-times of de Sitter universe and of Einstein universe are contained, are also spherically symmetric. Hence concerning the physical and mathematical properties of an S_0 many investigations have been made by many authors from various standpoints. In particular, in relativistic mechanics and cosmology, many physical properties of the S_0's of various types have been studied in detail basing upon the Einstein's field equation.[1] As regards the mathematical properties of an S_0 we have, for instance, a detailed research of Eiesland from the standpoint of continuous group of transformations.[2] Recently the present author has also made clear some geometrical properties of S_0 by introducing the concept of characteristic system of an S_0.[3]

In spite of these investigations, however, it seems to us that there exists no complete theory by which to determine whether a four dimensional Riemannian space V_4 defined by g_{ij} arbitrarily given in any coordinate system is spherically symmetric or not. If we express this problem mathematically it is 'to determine the necessary and sufficient condition that given g_{ij} be reducible to the form $(1\cdot1)$'.

On the other hand it is well known that, although at first sight a static axially symmetric solution of the Einstein's equation $K_{ij}=0$ obtained by the method of Weyl and Levi-Civita seems to be not spherically symmetric, we can transform it into the ordinary spherically symmetric form of the Schwarzschild's exterior solution. (See § 5). Contrary to this, as will also be seen in § 5, we can easily prove that the line elements of the space-times introduced by Gödel and by Silberstein can never be transformed into the form of (1·1) i.e. these two V_4's are not spherically symmetric.

As is seen from these examples, the problem of 'determining whether a given space-time is an S_0 or not' is only interesting from the standpoint of tensor analysis but also its solution is desirable from the physical standpoint. If the answer of this problem is given by the tensor equations to be satisfied by the curvature tensor K_{ijlm} made from g_{ij}, especially when the equations contain no tensor other than g_{ij}, ϵ_{ijlm} and K_{ijlm}, we may say that the problem is solved in the most desirable form. Since it is not easy to find such equations, however, it has not been succeeded as yet. In this paper we shall give another way of discriminating spherically symmetric space-times using the theory of the characteristic system of an S_0 introduced by the present author and finally in § 5, we shall apply this method to some kinds of space-times.

§ 2. Preliminaries

In this section, as the preparation of solving the problem stated in the introduction, we shall give the following new definition of an S_0 which was introduced by the present author and is equivalent to the ordinary one as was shown in [1]* :

A spherically symmetric space-time S_0 is a four dimensional Riemannian space having the following properties :

(I) Its curvature tensor satisfies the equation

$$K_{ijlm}=-\overset{1}{\rho}\,a_{[i}a_{[l}\beta_{j]}\beta_{m]}-\overset{2}{\rho}g_{[i[l}a_{j]}a_{m]}+\overset{3}{\rho}g_{[i[l}\beta_{j]}\beta_{m]}+\overset{4}{\rho}g_{[i[l}g_{j]m]}, \qquad (F_1)$$

where a_i and β_i are minus and plus unit vectors ($a_sa^s=-1$, $\beta_s\beta^s=1$) mutually orthogonal and satisfying

$$\nabla_i a_j=\sigma a_i\beta_j+\varkappa(g_{ij}+a_ia_j-\beta_i\beta_j)+\bar{\sigma}\beta_i\beta_j, \qquad (F_2)$$

$$\nabla_i\beta_j=\bar{\sigma}\beta_ia_j+\bar{\varkappa}(\quad,,\quad)+\sigma a_ia_j, \qquad (F_3)$$

and $\overset{a}{\rho}$ $(a=1,\ldots,4)$; σ, $\bar{\sigma}$; $\varkappa$, $\bar{\varkappa}$ are scalars determined from these equations.

(II) One of five scalars $\overset{a}{\rho}$ and $K\equiv K_{ij}{}^{ji}$ is such that its gradient vector is a linear combination of a_i and β_i.

(III) $$\overset{4}{\rho}-2(\varkappa^2-\bar{\varkappa}^2)\neq 0. \qquad (F_4)$$

(IV) The signature of the fundamental form is -2 i.e. is of type $(---+)$.

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* Throughout this paper we shall use the same notations as those in [1].

(α_i, β_i) and $(\overset{a}{\rho}, \sigma, \overline{\sigma}, \chi, \bar{\chi})$ are called characteristic vectors and scalars of the S_0 respectively and $(\alpha_i, \ldots, \bar{\chi})$ is generically called characteristic system and their properties are investigated in detail in [1]. Throughout this paper we shall use these results without stating them again.

Now let g_{ij} be an arbitrary fundamental tensor satisfying (IV) and V_4 be the space-time defined by this g_{ij}. To discriminate whether this V_4 is an S_0 or not we shall first determine from g_{ij} the forms to be taken by the characteristic vectors when the V_4 is assumed to be an S_0. If only this forms are obtained we can easily determine whether the V_4 is an S_0 or not by substituting them into the fundamental equations $(F_1), \ldots, (F_4)$ and testing whether the S_0 satisfies the conditions stated in the above new definition. We shall call such a way of discriminating the spherically symmetric property of a V_4 *c.v. test*. It is to be noticed that since an S_0 admits ϵ-transformation of the characteristic system* we can ignore the signs of the characteristic vectors in determining their forms.

§ 3. V_4's of types 0, I, II and III

In discriminating the V_4 we have first to compute the curvature tensor K_{ijlm} and Ricci tensor $K_{ij} \equiv K_{sij}^{\cdot\cdot\cdot s}$ from the given g_{ij}. Then by solving the equation

$$\det.|K_i^{\cdot j} - \nu\delta_i^j| = 0, \qquad (3\cdot1)$$

we can obtain four principal invariants of K_{ij}, $\nu_1, \ldots, \nu_4$, using which we shall classify V_4's into the following five kinds:

0:	V_4's whose ν's are of the form	(a, b, c, d), $(a, b, c, d \neq)$.
I:	,, ,,	(a, a, b, c), $(a, b, c \neq)$.
II:	,, ,,	(a, a, b, b), $(a \neq b)$.
III:	,, ,,	(a, a, a, b), $(a \neq b)$.
IV:	,, ,,	(a, a, a, a).

Of course this classification is independent of the special choice of the coordinate system.

When V_4 is of type **0:** Since $(3\cdot1)$ for any S_0 has at least one double root, this V_4 is not an S_0.

When V_4 is of type **I:** Let α_i and β_i be the minus and plus unit vectors in the principal directions of K_{ij} corresponding to b and c respectively. Then by making the c.v. test using these vectors we can determine whether the V_4 is an S_0 or not. (Of course when b or c gives null direction the V_4 is not spherically symmetric.) The proof is easy, so we shall omit it here.

When V_4 is of type **II:** This V_4 corresponds to S_a i.e. an S_0 whose $\overset{2}{\rho} = \overset{3}{\rho}$. Try the c.v. test using any pair of mutually orthogonal unit vectors in the 'Hauptgebiet' corresponding to a. If the V_4 passes the test it is an S_0, and if not we have to make similar c.v. test using b in place of a. If the V_4 succeeds in this new test it is an S_0 and if

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* Theorem [4.1] in [1].

not it is not an S_0. The proof is evident because an S_0 admits ω-transformation of the characteristic system.

When V_4 is of type ***III:*** Let β_i be the plus unit vector in the principal direction corresponding to b. If $\beta^s\Gamma_{sl}\beta^l \neq 0$, we have only to make the c.v. test taking the minus unit vector in the direction of this vector as α^i. Next, if $\beta^s\Gamma_{sl}\beta^l=0$, examine whether this β_i satisfies

$$K_{ijlm}=\overset{3}{\rho}\, g_{[i[l}\beta_{j]}\beta_{m]}+\overset{4}{\rho}\, g_{[i[l}g_{j]m]}, \qquad (\overset{3}{\rho}\neq 0), \tag{3·2}$$

and

$$\Gamma_{il}\beta_j=-\sigma(g_{ij}-\beta_i\beta_j) \tag{3·3}$$

or not.* When they are satisfied determine σ by $3\sigma=-\Gamma_{sl}\beta^s$, and if $dx^s\Gamma_{sl}\sigma=0$ holds for all dx^i orthogonal to β^i the V_4 is an S_0. When this procedure fails somewhere it is not an S_0.

Proof: The former part is obvious by the properties of an S_0 given in § 4 of [1]. Next when $\beta^s\Gamma_{sl}\beta^l=0$, if we assume that the V_4 is an S_0 we can easily show that its line element is reducible to

$$ds^2=-e^{2g(t)}(1+r^2/4R^2)^{-2}(dr^2+r^2d\theta^2+r^2\sin^2\theta\, d\phi^2)+dt^2, \tag{3·4}$$

and that the condition above stated is necessary. Conversely when the condition is satisfied, taking the geodesic congruence defined by β^i as parametric curves for $x^4\equiv t$ and its arc length as t we can prove that ds^2 is reducible to the form

$$ds^2=g_{ab}dx^adx^b+dt^2, \quad \beta_i=\beta^i=\delta^4_i, \quad g_{ab}=e^{2g(t)}\overset{*}{g}_{ab}(x^a), \quad (a, b=1, 2, 3), \tag{3·5}$$

and the three dimensional space defined by $\overset{*}{g}_{ab}dx^adx^b$ is of constant curvature. Hence our assertion is proved.

It is to be noticed that in the discriminating methods and their proofs given in this paper α_i and β_i may not necessarily be real though g_{ij} must always be real. But when the V_4 is an S_0 they become always real by taking a standard coordinate system for the characteristic system and making suitable i-transformation.

§ 4. V_4 of type IV

In this case it holds that

$$K_{ij}=(K/4)g_{ij}, \tag{4·1}$$

i.e. the V_4 is an Einstein space in the sense used in the differential geometry. In this section we shall give a method of discriminating such an Einstein space.

[a] When the V_4 satisfies $K_{ijlm}=\overset{4}{\rho}\, g_{[i[l}g_{j]m]}$, i.e. when the V_4 is of constant curvature, it is an S_0 evidently. (The de Sitter space-time.)

[b] When the V_4 is not of constant curvature. First, let us study some properties of such an S_0. If we put $K^{ij\cdot lm}_{\cdot\cdot}\equiv K^{\cdot A}_{A\cdot}$, $(A\equiv(i, j), B\equiv(l, m), A, B=1,\ldots, 6)$, six

* These two equations are obtained by studying the properties of an S_0 of type **III**.

principal invariants of K_{AB} are given by solving

$$\det.|K_A^{\cdot B}-\nu\,\delta_A^B|=0, \tag{4·2}$$

and as is shown in § 6 of [1] ν's must be of the type (a, a, a, a, ξ, ξ). When and only when ν's take the form $(0, 0, 0, 0, \eta, \eta)$, $(\eta=\text{const.})$, the S_0 is an S_{II} and otherwise it is an S_{15}, where both S_{II} and S_{15} are special kinds of S_0. ([1]).

[b_1] When the S_0 is an S_{15}, we can easily prove that ds^2 is reducible to

$$ds^2=-A(r)dr^2-r^2(d\theta^2+\sin^2\theta d\phi^2)+(1/A)dt^2,\ (A=(1-k^2r^2-2m/r)^{-1}), \tag{4·3}$$

where k^2 and $m(\neq 0)$ are arbitrary constants. Now putting

$$\mathfrak{R}_{ijlm}=K_{ij}^{\cdots pq}K_{pqlm},\qquad \mathfrak{R}_{ij}=\mathfrak{R}_{sij}^{\cdots\ \ s},\qquad \mathfrak{R}=\mathfrak{R}_s^{\cdot s}, \tag{4·4}$$

and using characteristic vectors $a_i=\sqrt{A}\,\delta_i$ and $\beta_i=(1/\sqrt{A})\,\delta_i^4$,* we have

$$K=12k^2,\qquad \mathfrak{R}=-24(k^2+2m^2/r^6), \tag{4·5}$$

$$\begin{cases} (\overset{2}{\rho})^2=-3(\mathfrak{R}+2K)\neq \text{const.},\quad \nabla_i(\log\overset{2}{\rho})=3\varkappa a_i,\quad 2\varkappa=\nabla_s a^s-\bar\sigma, \\ \nabla_i a_j=\varkappa(g_{ij}+a_ia_j)-(\varkappa-\bar\sigma)\beta_i\beta_j,\quad \bar\varkappa=\sigma=0,\quad (\varkappa-\bar\sigma\neq 0), \\ \overset{1}{\rho}=-2\overset{2}{\rho},\qquad \overset{2}{\rho}=\overset{3}{\rho},\qquad \overset{4}{\rho}=-(\overset{2}{\rho}+K/2)/3. \end{cases} \tag{4·6}$$

[b_2] When the S_0 is an S_{II}, by putting $\eta=-1/R^2$, ds^2 is reducible to

$$ds^2=(-dr^2+dt^2)\{1+(-r^2+t^2)/4R^2\}^{-2}-R^2(d\theta^2+\sin^2\theta d\phi^2), \tag{4·7}$$

and in this coordinate system we have the following two pairs of characteristic vectors mutually orthogonal:

$$a_j=\{1+(-r^2+t^2)/4R^2\}^{-1}\,\delta_j^1,\quad \beta_j=(\ \ ,,\ \ )^{-1}\,\delta_j^4, \tag{4·8}$$

$$\bar a_j=R\,\delta_j^2,\qquad \bar\beta_j=iR\,\sin\theta\,\delta_j^3, \tag{4·9}$$

where the second pair (4·9) is not real. For these vectors it holds that

$$P_{ij}^*\equiv\frac{1}{2}\epsilon_{ijlm}P^{lm}=-\bar P_{ij},\qquad \bar P_{ij}^*\equiv\frac{1}{2}\epsilon_{ijlm}\bar P^{lm}=-P_{ij}, \tag{4·10}$$

$$\begin{cases} P_{ij}P^{ij}=-\dfrac{1}{2}=\bar P_{ij}\bar P^{ij},\qquad P_{ij}\bar P^{ij}=0, \\ E\equiv\epsilon_{ijlm}P^{ij}P^{lm}=0,\quad F\equiv\epsilon_{ijlm}P^{ij}\bar P^{lm}=1,\quad G\equiv\epsilon_{ijlm}\bar P^{ij}\bar P^{lm}=0, \end{cases} \tag{4·11}$$

where $P_{ij}\equiv a_{[i}\beta_{j]}$, $\bar P_{ij}\equiv\bar a_{[i}\bar\beta_{j]}$, and ϵ_{ijlm} is the ϵ tensor. (Not tensor density. So $\epsilon_{1234}=\sqrt{g}=iR^2\{1+(-r^2+t^2)/4R^2\}^{-2}\sin\theta$ in this coordinate system.) Now let $2Q^A$ and $2\bar Q^A$ be any minus unit vectors mutually orthogonal in the Hauptgebiet corresponding to $-1/R^2$, then we have

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* Since an S_{15} admits ω-transformation there always exist such characteristic vectors.

$$Q^A = P^A \cos\omega - \bar{P}^A \sin\omega, \quad \bar{Q}^A = P^A \sin\omega + \bar{P}^A \cos\omega, \quad (P^A \equiv P^{ij},\ \bar{P}^A \equiv \bar{P}^{ij}), \tag{4·12}$$

$$\left\{\begin{array}{l} E' \equiv \epsilon_{ijlm} Q^{ij} Q^{lm} = -\sin 2\omega, \quad F' \equiv \epsilon_{ijlm} Q^{ij} \bar{Q}^{lm} = \cos 2\omega, \\ G' \equiv \epsilon_{ijlm} \bar{Q}^{ij} \bar{Q}^{lm} = \sin 2\omega, \quad (Q^{ij} \equiv Q^A, \quad \bar{Q}^{ij} \equiv \bar{Q}^A), \end{array}\right. \tag{4·13}$$

where ω is a parameter. Conversely P^A and $\bar{P}^A$ are determined from Q^A and $\bar{Q}^A$.

On the other hand we can easily prove that:

Lemma A necessary and sufficient condition that a pair of unit vectors α_i and β_i satisfying $-\alpha_s\alpha^s = \beta_s\beta^s = 1$, $\alpha_s\beta^s = 0$ and $2\,\alpha_{[i}\beta_{j]} = p_{ij}$, $(p_{ij} = -p_{ji})$, exist is given by

$$\epsilon_{ijlm} p^{ij} p^{lm} = 0, \qquad p_{ij} p^{ij} = -2. \tag{4·14}$$

When this condition is satisfied the vectors are determined to within their signs and a pseudo-orthogonal transformation.

Using this lemma and the results obtained in this section we have the following way of determining whether a V_4 of the type **IV** which is not of constant curvature is an S_0 or not:

When ν's are not of the form $(\alpha, \alpha, \alpha, \alpha, \xi, \tilde{\xi})$, $(\alpha \neq \tilde{\xi})$, the V_4 is not an S_0.

When ν's are of this form and not of the form $(0, 0, 0, 0, \eta, \eta)$, $(\eta = \text{const.})$, compute K and $\mathfrak{R}$. Then K must constant. Determine $\overset{2}{\rho}$, α_i, $\varkappa$ and β_i in turn by (4·6). Then we have only to make the c.v. test using α_i and β_i thus obtained. If the V_4 succeeds in all tests it is the S_{15} defined by (4·3) i.e. Schwarzschild-de Sitter space-time. If this procedure fails somewhere the V_4 is not an S_0.

Next when ν's are of the form $(0, 0, 0, 0, -1/R^2, -1/R^2)$, take any pair of minus unit vectors $2Q^A$ and $2\bar{Q}^A$ mutually orthogonal in the Hauptgebiet corresponding to $-1/R^2$ and calculate E', F' and G'. Determine ω from (4·13) and put

$$P^A = Q^A \cos\omega + \bar{Q}^A \sin\omega, \quad \bar{P}^A = -Q^A \sin\omega + \bar{Q}^A \cos\omega. \tag{4·15}$$

Then (4·11) must hold for these P^A and $\bar{P}^A$. From both P_{ij} and $\bar{P}_{ij}$ we can obtain (α_i, β_i) by virtue of the lemma. Then we have only to make the c.v. test using the vectors obtained from P_{ij}. If the V_4 passes the test it must also pass the test for the other pair obtained from $\bar{P}_{ij}$, and the V_4 is an S_{11} defined by (4·7). If this procedure fails somewhere it is not an S_0.

In this S_{11} it holds that

$$\begin{aligned} &\overset{1}{\rho} = -2\overset{2}{\rho} = -2\overset{3}{\rho} = 4\overset{4}{\rho} = -2K = -8/R^2, \\ &\mathfrak{R}_{ijlm} = -(2/R^2) K_{ijlm}, \end{aligned} \tag{4·16}$$

and for the real characteristic vectors (4·8),

$$\sigma = \varkappa = \bar{\varkappa} = 0, \qquad \bar{\sigma} = -\cot\theta/R. \tag{4·17}$$

§ 5. Some examples

[a] *Gödel's space-time* Gödel obtained the following line element as a cosmological solution of Einstein's field equation:[4]

$$ds^2=a^2\{-(dx^1)^2+(e^{2x^1}/2)(dx^2)^2-(dx^3)^2+2e^{x^1}dx^2dx^4\}, \tag{5·1}$$

where a is a positive constant. Now as an application of our theory, we shall show that the V_4 defined by (5·1) is not an S_0. Non-vanishing components of the Ricci tensor made from (5·1) are given by

$$K_{22}=-e^{2x^1}, \quad K_{44}=-1, \quad K_{24}=K_{42}=-e^{x^1}. \tag{5·2}$$

Hence the four principal invariants of K_{ij} are 0, 0, 0 and $1/a^2$ and this V_4 is of type **III.** β^i corresponding to $\nu=1/a^2$ is given by

$$\beta^i=(0, 0, 0, 1/a), \qquad \text{so} \qquad \beta_i=(0, ae^{x^1}, 0, a), \tag{5·3}$$

from which we have $\beta^s\nabla_s\beta^i=0$ and moreover we can easily show that (3·3) is not satisfied by this β^i. Therefore this V_4 is not an S_0.

[b] *The space-time of Weyl and Levi-Civita* By the method of Weyl and Levi-Civita we can obtain the following static and axially symmetric solution of the Einstein's field equation $K_{ij}=0$.[5]

$$ds^2=-e^{2(\lambda-\psi)}(d\rho^2+dz^2)-\rho^2e^{-2\psi}d\phi^2+e^{2\psi}dt^2. \tag{5·4}$$

where $\psi=\psi(\rho, z)$ is any solution of

$$\Delta\psi\equiv(\rho\psi')'+\bar{\bar{\psi}}=0, \tag{5·5}$$

and $\lambda=\lambda(\rho, z)$ is obtained by solving

$$d\lambda=\rho(\psi'^2-\bar{\psi}^2)\,d\rho+2\rho\psi'\bar{\psi}dz, \tag{5·6}$$

where a prime and a bar denote partial derivatives with respect to ρ and z respectively. Now we shall take the special case in which

$$\begin{aligned}\psi&=\frac{1}{2}\log(r_1+r_2-2m)/(r_1+r_2+2m),\\ \lambda&=\frac{1}{2}\log[\{(r_1+r_2)^2-4m^2\}/4r_1r_2],\end{aligned} \tag{5·7}$$

where m is any constant and $r_1=\sqrt{\{\rho^2+(z-m)^2\}}$, and $r_2=\sqrt{\{\rho^2+(z+m)^2\}}$. At first sight it seems that this V_4 is not spherically symmetric. It is well known, however, that this V_4 is nothing but the spherically symmetric space-time of Schwarzschild's exterior solution. In fact the line element (5·4) with (5·7) is transformed into the ordinary form

$$ds^2=-(1-2m/r)^{-1}dr^2-r^2(d\theta^2+\sin^2\theta\,d\phi^2)+(1-2m/r)dt^2 \tag{5·8}$$

by the coordinate transformation

$$r=m+(r_1+r_2)/2, \qquad \cos\theta=(r_1-r_2)/2m. \tag{5·9}$$

Now, we shall apply our present theory to the g_{ij} of the form (5·4) with (5·7). In this case, from $K_{ij}=0$ we know that the V_4 is of type **IV**. In general, non-vanishing components of $K_{ij}^{\cdot\cdot lm}$ for (5·4) with (5·5) and (5·6) are given by

$$\begin{aligned}
&\mu_1 \equiv K_{12}^{\cdot\cdot 12}=K_{34}^{\cdot\cdot 34}=(\psi'/\rho-\psi'^2-\bar{\psi}^2)e^{-2(\lambda-\Psi)},\\
&\mu_2 \equiv K_{13}^{\cdot\cdot 13}=K_{24}^{\cdot\cdot 24}=-(\psi''+\psi'/\rho+\psi'^2-2\bar{\psi}^2-\rho\psi'^3+3\rho\psi'\bar{\psi}^2)e^{-2(\lambda-\Psi)},\\
&\mu_3 \equiv K_{14}^{\cdot\cdot 14}=K_{23}^{\cdot\cdot 23}=(\psi''+\psi'^2-\bar{\psi}^2-\rho\psi'^3+3\rho\psi'\bar{\psi}^2)e^{-2(\lambda-\Psi)},\\
&\mu_4 \equiv -K_{13}^{\cdot\cdot 23}=K_{14}^{\cdot\cdot 24}=(\bar{\psi}'+3\psi'\bar{\psi}-3\rho\psi'^2\bar{\psi}+\rho\bar{\psi}^3)e^{-2(\lambda-\Psi)}.
\end{aligned} \tag{5·10}$$

Solutions of (4·2) are given by

$$\nu=(\mu_1,\ \mu_1,\ \bar{\mu}_1,\ \bar{\mu}_1,\ \bar{\mu}_2,\ \bar{\mu}_2), \tag{5·11}$$

where $\bar{\mu}_1$ and $\bar{\mu}_2$ are two roots of the equation

$$\mu^2-\mu(\mu_2+\mu_3)+\mu_2\mu_3-\mu_4^2=0. \tag{5·12}$$

If we substitute (5·7) into (5·10) we have

$$\begin{aligned}
&\mu_1=m/r^3,\quad \mu_2=-m(2a-b)e^{2(\lambda-\Psi)}/r^5,\quad \mu_3=m(a-2b)e^{2(\lambda-\Psi)}/r^5,\\
&\mu_4=3m\rho(r-m)e^{2(\lambda-\Psi)}\cos\theta/r^5 \neq 0,\qquad \begin{pmatrix} a=r^2(1-2m/r)\cos^2\theta,\\ b=(r-m)^2\sin^2\theta \end{pmatrix},
\end{aligned} \tag{5·13}$$

where r and θ are used. Hence this V_4 is not of constant curvature. Furthermore we can easily prove that μ_1 satisfies (5·12) and that (5·12) has no double root. Hence principal invariants of K_{AB} are of the form $(\mu_1,\ \mu_1,\ \mu_1,\ \mu_1,\ \bar{\mu}_2,\ \bar{\mu}_2)$, $(\mu_1 \neq \bar{\mu}_2)$. Then by the method stated in § 4, we can easily prove that this V_4 is the S_{15} defined by (5·8).

[c] *Silberstein's space-time of single mass center* Next we shall give an example of V_4 which is also an axially symmetric static solution of $K_{ij}=0$ but is not an S_0. Silberstein obtained the following solution of (5·5) and (5·6) :[6]

$$\psi=-L/r,\quad \lambda=-L^2\rho^2/2r^4,\quad (r^2=\rho^2+z^2), \tag{5·14}$$

where L is an arbitrary constant and called this single mass solution. Of course this V_4 is also of type **IV**. Substituting (5·14) into (5·10), we have

$$\begin{aligned}
&\mu_1=(Lr^{-3}-L^2r^{-4})e^{2(\Psi-\lambda)},\\
&\mu_2=\{L(-2r^{-3}+3\rho^2r^{-5})+L^2(-\rho^2+2z^2)r^{-6}+L^3\rho^2(\rho^2-3z^2)r^{-9}\}e^{2(\Psi-\lambda)},\\
&\mu_3=\{L(r^{-3}-3\rho^2r^{-5})+L^2(2\rho^2-z^2)r^{-6}-L^3\rho^2(\rho^2-3z^2)r^{-9}\}e^{2(\Psi-\lambda)},\\
&\mu_4=\{-3Lr^{-5}+3L^2r^{-6}+L^3(-3\rho^2+z^2)r^{-9}\}\rho z e^{2(\Psi-\lambda)},
\end{aligned} \tag{5·15}$$

using which we can prove that the ν's are of the form $(a,\ a,\ b,\ b,\ c,\ c)$, $(a,\ b,\ c \neq)$. Hence this V_4 is not an S_0.

§ 6. Conclusion

Spherically symmetric space-times are treated frequently in the general theory of relativity. It seems to the author, however, that in usual theory more importance is

attached to the special forms of their line elements in some coordinate systems than to their intrinsic properties. The general theory of relativity is a theory of analytical invariants from the mathematical standpoint and this fact is one of the characteristic features of the theory. Hence it will not be meaningless to take the view-point that a space-time is a geometrical entity independent of the special choice of the coordinate system and to deal with its spherical symmetry as their intrinsic property. The present paper as well as the earlier papers of the author [1], etc.[3] has been written along this line of thought, and a theory concerning the discrimination of the spherically symmetric space-times has been constructed. Although it is not of the ideal form, we can determine by it whether a four dimensional Riemannian space defined by an arbitrarily given g_{ij} is spherically symmetric or not. Accordingly we may say that we have succeeded in advancing a step further.

Hereafter when a new space-time which is apparently not spherically symmetric is introduced, we hope that the method given in the present paper may be applied to determine whether it is spherically symmetric or not.

Appendix

[a] For an S_0, the following relations hold:

$$\begin{aligned}
\mathfrak{R}_{ijlm} &= -\frac{1}{2}\left\{(\overset{1}{\rho})^2+2\overset{1}{\rho}(\overset{2}{\rho}+\overset{3}{\rho})+4\overset{1}{\rho}\overset{4}{\rho}+\overset{2}{\rho}\overset{3}{\rho}\right\}P_{ij}P_{lm}-\frac{1}{2}\overset{2}{\rho}(\overset{2}{\rho}+4\overset{4}{\rho})A_{ijlm}\\
&\quad+\frac{1}{2}\overset{3}{\rho}(\overset{3}{\rho}+4\overset{4}{\rho})B_{ijlm}+(\overset{4}{\rho})^2G_{ijlm},\\
\mathfrak{R}_{jl} &= \frac{1}{8}\left\{(\overset{1}{\rho})^2+2\overset{1}{\rho}(\overset{2}{\rho}+\overset{3}{\rho})+2\overset{2}{\rho}\overset{3}{\rho}+4\overset{1}{\rho}\overset{4}{\rho}+2\overset{2}{\rho}(\overset{2}{\rho}+4\overset{4}{\rho})\right\}u_ju_l\\
&\quad-\frac{1}{8}\left\{(\overset{1}{\rho})^2+2\overset{1}{\rho}(\overset{2}{\rho}+\overset{3}{\rho})+2\overset{2}{\rho}\overset{3}{\rho}+4\overset{1}{\rho}\overset{4}{\rho}+2\overset{3}{\rho}(\overset{3}{\rho}+4\overset{4}{\rho})\right\}\beta_j\beta_l \qquad \text{(A·1)}\\
&\quad-\frac{1}{8}\left\{\overset{2}{\rho}(\overset{2}{\rho}+4\overset{4}{\rho})+\overset{3}{\rho}(\overset{3}{\rho}+4\overset{4}{\rho})+12(\overset{4}{\rho})^2\right\}g_{jl},\\
\mathfrak{R} &= -\frac{1}{4}\left\{(\overset{1}{\rho})^2+2\overset{1}{\rho}(\overset{2}{\rho}+\overset{3}{\rho})+2\overset{2}{\rho}\overset{3}{\rho}+4\overset{1}{\rho}\overset{4}{\rho}+3\overset{2}{\rho}(\overset{2}{\rho}+4\overset{4}{\rho})+3\overset{3}{\rho}(\overset{3}{\rho}+4\overset{4}{\rho})+24(\overset{4}{\rho})^2\right\},
\end{aligned}$$

where $A_{ijlm}=g_{[i[l}u_{j]}u_{m]}$, $B_{ijlm}=g_{[i[l}\beta_{j]}\beta_{m]}$ and $G_{ijlm}=g_{[i[l}g_{j]m]}$.

In the same way we can express the scalars peculiar to the S_0 e.g., K, $K_{ij}K^{ij}$, $K_{ijkl}K^{ijkl}$, $K_{ij}\mathfrak{R}^{ij}$,... in terms of ρ's, and conversely by solving these equations we can express ρ's in terms of K, $\mathfrak{R}$,... For example,

$$(\overset{1}{\rho})^2=4(K)^2-12(\mathfrak{R}+2K_{ij}K^{ij}), \qquad \text{(A·2)}$$

and $\overset{2}{\rho}$, $\overset{3}{\rho}$, $\overset{4}{\rho}$ are given by solving

$$m=-(2K+\overset{1}{\rho})/3-4\overset{4}{\rho},\quad 8n=2(\overset{1}{\rho})^2+2\overset{1}{\rho}m+3m^2+4(3\mathfrak{R}+2K_{ij}K^{ij}),$$
$$\mathfrak{R}_{ij}K^{ij}=\text{Polynomial of }(m,\ n,\ \overset{4}{\rho}), \tag{A·3}$$

where $m=\overset{2}{\rho}+\overset{3}{\rho}$ and $n=\overset{2}{\rho}\overset{3}{\rho}$. Since g_{ij} is invariant under any motion, these scalars K, $\mathfrak{R}$, $K_{ij}K^{ij}$, etc. are also invariant under any m-transformation. (See [1].) Hence we have the important result:

Theorem *ρ's are invariant under any m-transformation.*

[b] We can generalize the results obtained in this paper in n ($n>4$) dimensional case by modifying suitably. But it must be noticed that in solving (3·1) or (4·2) in n dimensional case there is no need of solving third or higher order equation directly, because we start with the examination of multiple root.

References

1) For example, see R. C. Tolman, *Relativity, Thermodynamics and Cosmology*, Oxford (1934).
2) J. Eiesland, Trans. Amer. Math. Soc. **27** (1925), 213.
3) H. Takeno, Journ. Math. Soc. Japan **3** (1951), 317. This paper is cited as [1].
H. Takeno, Journ. Sci. Hiroshima Univ. **16** (1952), 67. Another two papers are in the press on the same Journal. See also
H. Takeno, Journ. Sci. Hiroshima Univ. **12** (1942), 126 (in Japanese).
4) K. Gödel, Rev. Mod. Phys. **21** (1949), 447.
5) H. Weyl, Ann. d. Phys. **54** (1918), 117; **59** (1919), 185;
T. Levi-Civita, Rend. Acc. d. Lincei (1919);
R. Bach and Weyl, Math. Zeits. **13** (1922), 134. See also
N. Rosen, Rev. Mod. Phys. **21** (1949), 503.
6) L. Silberstein, Phys. Rev. **49** (1936), 208.

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The Quantum-Statistical Theory of Transport Phenomena, I*

—— *On the Boltzmann-Uehling-Uhlenbeck Equation* ——

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By means of the N-representation of density operator, Irving and Zwanzig's equation of motion for the phase-space distribution function is rewritten in such a form that the influence of the symmetry effect appears more explicitly in the collision term of the equation for the singlet distribution function. By means of the customary theory of time-dependent perturbation, the equation of motion for the time averaged distribution function over an interval as long as the mean life of the unperturbed quantum states, is derived from the Irving-Zwanzig equation. This equation is compared with the Uehling-Uhlenbeck equation, which is obtained as the quantum mechanical modification of the Boltzmann integro-differential equation by means of a physical argument. (Then, it is concluded that the deviation from the Uehling-Uhlenbeck equation becomes important if that the local variation of the external field or of the distribution function in the range of the order of the magnitude of the de Broglie wave length is appreciable.) And it seems probable that the Uehling-Uhlenbeck equation becomes invalid at extremely low temperatures, such as the λ-point of liquid helium. We have, however, not succeeded in the derivation of an equation for the general case, because the postulate of random *a priori* phases destroys the dependence of the initial distribution on coordinates.

§ 1. Introduction

About twenty years ago, Uehling and Uhlenbeck[1] established the fundamental equation for quantum theory of transport properties in gases of low density, by means of a physical argument which would seem to be plausible. In spite of rather obscure points left in Uehling and Uhlenbeck's derivation, the subsequent theories on transport in quantum liquids had been based on this equation, until Irving and Zwanzig[2] recently established the equation of motion for the phase-space distribution function (Hereafter we will abbreviate the distribution function to d.f.) first introduced by Wigner[3]. The Irving-Zwanzig equation, which is obtained as the Fourier-transform of the quantum-mechanical Liouville equation, should be considered as the starting point for the theory on transport in quantum fluids.

On the other hand, Kirkwood[4] has succeeded in analytical derivation of the classical Boltzmann equation from the principles of statistical mechanics, by using the time averaging procedure over a certain interval of time. With such a procedure, we shall here

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attempt to derive the equation of motion for the time-averaged Wigner d.f. In performing the time average, the customary theory of time-dependent perturbation theory will be employed, though the result may be obtained by an alternative method shown in appendix. In the last section, deviation from the Uehling-Uhlenbeck equation will be discussed in detail.

§ 2. The N-representation

We consider a system composed of N identical Bose or Fermi particles. And let q^N be the set of coordinates of the system and q_i be the set of coordinates of the i-th particle; coordinates mean both spatial and spin coordinates. It is well known that the Gibbs ensemble of quantum-mechanical system can be described by the density operator first introduced by von Neumann[5]. This operator is defined as

$$\boldsymbol{\rho}=\sum_j w_j \boldsymbol{P}[\Phi_j(q^N, t)] \tag{2·1}$$

with

$$\sum_j w_j=1 \qquad \text{and} \qquad w_j \geq 0,$$

where $\{\Phi_j(q^N, t)\}$ is an orthonormal set of wave functions, w_j is the probability of the system being in the j-th state, and $\boldsymbol{P}[\Phi_j]$ is a projection operator of Φ_j. The dependence of the density operator on time is given by the quantum-mechanical Liouville equation,

$$d\boldsymbol{\rho}/dt=\partial\boldsymbol{\rho}/\partial t+[\boldsymbol{\rho H}-\boldsymbol{H\rho}]/i\hbar=0, \tag{2·2}$$

$\boldsymbol{H}$ being the Hamiltonian of the system.

Let $\{\psi_t(q)\}$ be an orthonormal set of functions of coordinates of single particle, and then one of the orthonormal sets of functions of q^N, which are symmetric or antisymmetric in the permutations of the coordinates of all particles, is given by

$$\Psi^{(\pm)}_{n_1, n_2, \cdots}(q^N)=\det{}^{(\pm)}[\psi_{t_1}(q_1)\cdots\psi_{t_N}(q_N)], \tag{2·3}$$

where $\det^{(+)}$ and $\det^{(-)}$ indicate a permanent and a determinant, respectively. The transformed wave function in the N-representation, $C_j(\{n_t\}, t)$, is defined by

$$\Phi_j(q^N, t)=\sum_{\substack{\{n_t\} \\ [\sum_t n_t=N]}} C_j(\{n_t\}, t)\ \Psi^{(\pm)}_{\{n_t\}}(q^N), \tag{2·4}$$

where n_t is the number of particles in the state represented by $\psi_t(q)$. Then the matrix element of $\boldsymbol{\rho}$ in the N-representation can be written as

$$\rho^{(N)}(\varkappa, \varkappa'; t)=\sum_j w_j C_j^*(\varkappa', t) C_j(\varkappa, t), \tag{2·5}$$

where $\varkappa$ represents a set of integers $\{n_t\}$.

Using annihilation operators a_t and creation operators a_t^*, which are conjugate to each other and both of which act upon $\Psi^{(\pm)}_{\{n_t\}}(q)$, we can write the Hamiltonian $\boldsymbol{H}=\sum_i A(q_i)+\sum_{i>j} u(q_i, q_j)$ in the form[6]

$$\boldsymbol{H}=\sum_{t}\sum_{\bar{t}} a_t^* a_{\bar{t}} \int \psi_t^*(q) A(q) \psi_{\bar{t}}(q) dq$$

$$+\frac{1}{2}\sum_{t}\sum_{u}\sum_{\bar{t}}\sum_{\bar{u}} a_t^* a_u^* a_{\bar{u}} a_{\bar{t}} \iint \psi_t^*(q_1)\psi_u^*(q_2) u(q_1, q_2)\psi_{\bar{t}}(q_1)\psi_{\bar{u}}(q_2) dq_1 dq_2. \quad (2\cdot 6)$$

The reduced density matrices in the q-representation are given by[7]

$$\rho^{(n)}(q_1,\cdots, q_n;\ q_1',\cdots, q_n';\ t)$$

$$=[N!/(N-n)!]\int^{(N-n)}\cdots\int \rho^{(N)}(q_1,\cdots, q_n, \bar{q}_{n+1},\cdots,\bar{q}_N;\ q_1',\cdots, q_n', \bar{q}_{n+1},\cdots,\bar{q}_N;\ t)$$

$$\cdot d\bar{q}_{n+1}\cdots d\bar{q}_N$$

$$=\sum_{\varkappa} \boldsymbol{\psi}^*(q_1')\cdots\boldsymbol{\psi}^*(q_n')\boldsymbol{\psi}(q_n)\cdots\boldsymbol{\psi}(q_1)\rho^{(N)}(\varkappa,\varkappa;t), \quad (2\cdot 7)$$

where $\boldsymbol{\psi}(q)$ is the quantized wave function:

$$\boldsymbol{\psi}(q)=\sum_{t} a_t \psi_t(q), \quad (2\cdot 8)$$

operating on the first index $\varkappa$ of the density matrix,

$$\rho^{(N)}(\varkappa,\varkappa';t)=\iint \Psi_{\varkappa}^{(\pm)*}(q^N)\ \rho^{(N)}(q^N, q'^N;t)\ \Psi_{\varkappa'}^{(\pm)}(q'^N) dq^N dq'^N, \quad (2\cdot 9)$$

which is an alternative expression for $(2\cdot 5)$. The calculations in the subsequent sections are carried out only for the case of the Bose-Einstein statistics, but the calculations for the Fermi-Dirac case can be done in the same manner.

§ 3. The phase-space distribution

The phase-space d.f. first introduced by Wigner[3] was extensively investigated by Moyal[8] for a pure state and was applied to quantum hydrodynamics by Irving and Zwanzig[2]. The d.f. in the phase space is defined, in terms of the density matrix in coordinate or momentum representation, as follows:

$$f^{(N)}(X, P, t)=h^{-3N}\int^{(N)}\cdots\int e^{P\cdot Y/i\hbar}\rho^{(N)}\left(X-\frac{1}{2}Y, X+\frac{1}{2}Y;t\right)dY \quad (3\cdot 1)$$

$$=h^{-3N}\int^{(N)}\cdots\int e^{Q\cdot X/i\hbar}\rho^{(N)}\left(P-\frac{1}{2}Q, P+\frac{1}{2}Q;t\right)dQ, \quad (3\cdot 2)$$

where X and P are respectively the sets of the spatial coordinates $(x_1,\cdots, x_N)$ and momenta $(p_1,\cdots, p_N)$ of N particles, and $P.Y=\sum_{i=1}^{N}\boldsymbol{p}_i\cdot\boldsymbol{x}_i$. In the present and the subsequent sections, the momentum is often considered to have discrete spectrum, but no alteration in the formalism is necessary if one only introduces the Fourier-Stieltjes integral instead of the ordinary Fourier integral[9]. Integration over configurational or momentum space immediately gives

$$\int f^{(N)}(X, P, t)dX=\rho^{(N)}(P, P; t), \tag{3·3}$$

or

$$\int f^{(N)}(X, P, t)dP=\rho^{(N)}(X, X; t). \tag{3·4}$$

It may be observed from (3·2) that the dependence of the phase-space d.f. on the coordinates is furnished from a Fourier inversion of non-diagonal elements of the density matrix in the momentum representation. This fact arises from the wave nature of particles, mathematically expressed by the Fourier transform relation between coordinate and momentum representations.

The reduced phase-space d.f. is defined as

$$\begin{aligned} &f^{(n)}(\boldsymbol{x}_1,\cdots,\ \boldsymbol{x}_n\,;\boldsymbol{p}_1,\cdots,\ \boldsymbol{p}_n\,;t)\\ &=\int^{(N-n)}\cdots\int f^{(N)}(\boldsymbol{x},\ \bar{\boldsymbol{x}}_{n+1},\cdots,\ \bar{\boldsymbol{x}}_N\,;\ \boldsymbol{p},\ \bar{\boldsymbol{p}}_{n+1},\cdots,\bar{\boldsymbol{p}}_N\,;\ t)\ d\bar{\boldsymbol{x}}_{n+1}\cdots d\bar{\boldsymbol{x}}_N\,d\bar{\boldsymbol{p}}_{n+1}\cdots d\bar{\boldsymbol{p}}_N\\ &=h^{-3n}[(N-n)!/N!]\int^{(n)}\cdots\int e^{-p\cdot y/i\hbar}\rho^{(n)}\Big(\boldsymbol{x}_1-\frac{1}{2}\boldsymbol{y}_1,\cdots,\boldsymbol{x}_n-\frac{1}{2}\boldsymbol{y}_n\,;\ \boldsymbol{x}_1\\ &\qquad\qquad+\frac{1}{2}\boldsymbol{y}_1,\cdots,\boldsymbol{x}_n+\frac{1}{2}\boldsymbol{y}_n\,;\ t\Big)d\boldsymbol{y}. \end{aligned} \tag{3·5}$$

The equation of motion for $f^{(N)}$ is obtained as a Fourier inversion of the quantum-mechanical Liouville equation for the density matrix in the coordinate representation :

$$\partial f^{(N)}/\partial t+\sum_{i=1}^{N}(\boldsymbol{p}_i/m)\cdot\nabla_{x_i}f^{(N)}=(2/\hbar)\sin[(\hbar/2)\nabla_X\cdot\nabla_P]\,U(X)f^{(N)}, \tag{3·6}$$

where $U(X)=\sum_{i=1}^{N}u^{(e)}(\boldsymbol{x}_i)+\sum_{i>j}u(\boldsymbol{x}_i,\boldsymbol{x}_j)$ is the potential energy of the system and $\nabla_X=\sum_i\nabla_{x_i}$ operates only on the potential energy. The equation of motion for $f^{(n)}$ is obtained by integrating (3·6) with respect to the coordinates and momenta of the remaining $N-n$ particles. For the singlet phase-space d.f., we have

$$\begin{aligned} &\partial f^{(1)}/\partial t+(\boldsymbol{p}_1/m)\cdot\nabla_{x_1}f^{(1)}+\theta_1^{(e)}f^{(1)}\\ &\qquad=-\sum_{j=2}^{N}\iint\theta_{1j}f^{(2)}(\boldsymbol{x}_1,\boldsymbol{x}_j\,;\boldsymbol{p}_1,\boldsymbol{p}_j\,;t)\ d\boldsymbol{x}_j\,d\boldsymbol{p}_j\,, \end{aligned} \tag{3·7}$$

in which

$$\theta_1^{(e)}f^{(1)}=-(2/\hbar)\sin[(\hbar/2)\nabla_{x_1}\cdot\nabla_{p_1}]\,u^{(e)}(\boldsymbol{x}_1)\,f^{(1)}(\boldsymbol{x}_1,\boldsymbol{p}_1,t) \tag{3·8}$$

and

$$\begin{aligned} \theta_{1j}f^{(2)}=&-[1/N(N-1)i\hbar](1/\hbar\pi)^3\int\cdots\int d\bar{\boldsymbol{x}}_1d\bar{\boldsymbol{x}}_j\,u(\bar{\boldsymbol{x}}_1,\bar{\boldsymbol{x}}_j)\\ &\times[\exp(-2\{\boldsymbol{p}_1\cdot(\boldsymbol{x}_1-\bar{\boldsymbol{x}}_1)+\boldsymbol{p}_j\cdot(\boldsymbol{x}_j-\bar{\boldsymbol{x}}_j)\}/i\hbar)\\ &\times\rho^{(2)}(\bar{\boldsymbol{x}}_1,\bar{\boldsymbol{x}}_j\,;2\boldsymbol{x}_1-\bar{\boldsymbol{x}}_1,2\boldsymbol{x}_j-\bar{\boldsymbol{x}}_j\,;t)-c.c.], \end{aligned} \tag{3·9}$$

where ∇_x operates only on the potential energy. $\theta_1^{(e)} f^{(1)}$ is the term due to the external field and $\theta_{1j} f^{(2)}$'s are the terms due to the interaction between particles.

Choosing the orthonormal set of plane waves, $h^{-3/2} \exp(-\boldsymbol{p}\cdot\boldsymbol{x}/i\hbar)$, we have

$$\rho^{(2)}(\overline{\boldsymbol{x}}_1, \overline{\boldsymbol{x}}_j; 2\boldsymbol{x}_1-\overline{\boldsymbol{x}}_1, 2\boldsymbol{x}_j-\overline{\boldsymbol{x}}_j; t)$$
$$= h^{-6} \mathbf{S}_{p,q,r,s} g^{(2)}(pq, rs; t) \exp[-\{(\boldsymbol{p}_r+\boldsymbol{p}_p)\cdot\overline{\boldsymbol{x}}_1 + (\boldsymbol{p}_s+\boldsymbol{p}_q)\cdot\overline{\boldsymbol{x}}_j - 2\boldsymbol{p}_p\cdot\boldsymbol{x}_1 - 2\boldsymbol{p}_q\cdot\boldsymbol{x}_j\}/i\hbar], \quad (3\cdot10)$$

with

$$g^{(2)}(pq, rs; t) = a_p^* a_q^* a_r a_s, \quad (3\cdot11)$$

where p, q, r, and s indicate the discrete eigenvalues of momentum $\boldsymbol{p}$, which may be considered as continuous in the limit, and $\mathbf{S}$ represents the summation over them. Substituting the expression (3·10) for $\rho^{(2)}$ into (3·9) and integrating with respect to $\overline{\boldsymbol{x}}_1$, $\overline{\boldsymbol{x}}_j$, and $\boldsymbol{x}_j$, one obtains

$$\partial f^{(1)}/\partial t + (\boldsymbol{p}_1/m)\cdot\nabla_{x_1} f^{(1)} + \theta_1^{(e)} f^{(1)} = \{T_1 + T_1^*\}/N, \quad (3\cdot12)$$

where

$$T_1 = (1/i\hbar\cdot h^6)\int d\boldsymbol{p}_2 \mathbf{S}\, g^{(2)}(pq, rs, t)\, I(2, s) \exp[-2(\boldsymbol{p}_1-\boldsymbol{p}_p)\cdot\boldsymbol{x}_1/i\hbar]$$
$$\times \delta(\boldsymbol{p}_2-\boldsymbol{p}_q)\cdot\delta\Big(\boldsymbol{p}_1+\boldsymbol{p}_2-\frac{1}{2}(\boldsymbol{p}_p+\boldsymbol{p}_q+\boldsymbol{p}_r+\boldsymbol{p}_s)\Big) \quad (3\cdot13)$$

and

$$I(2, s) = 4\pi\int_0^\infty [\sin(pr/\hbar)/(pr/\hbar)]\, u(r) r^2 dr, \quad p = |\boldsymbol{p}_2-\boldsymbol{p}_s|. \quad (3\cdot14)$$

T_1 is a function of both $\boldsymbol{p}_1$ and $\boldsymbol{x}_1$, and terms for $p=r$, $q=s$ and $p=s$, $q=r$ are purely imaginary and independent on $\boldsymbol{x}_1$. Thus only the non-diagonal elements of $g^{(2)}$ contribute to the collision term and at the same time give the $\boldsymbol{x}_1$-dependence of T_1.

§ 4. The time average over a microscopic interval of time

Kirkwood[4] has derived the Boltzmann integro-differential equation by time averaging the equation for the singlet d.f. obtained from the classical Liouville equation. In the present paper, we shall attempt to derive the Uehling-Uhlenbeck integro-differential equation from the Irving-Zwanzig equation (3·7), which is the starting point for a quantum-statistical theory of transport, by time averaging over a finite interval in the same manner as in Kirkwood's theory of transport in classical statistical mechanics. This time averaging is denoted by a bar so that the time averaged phase-space d.f. is $\bar{f}^{(1)}$. Thus, one obtains from (3·12)

$$\partial\bar{f}^{(1)}/\partial t + (\boldsymbol{p}_1/m)\cdot\nabla_{x_1}\bar{f}^{(1)} + \theta_1^{(e)}\bar{f}^{(1)} = \{T_1 + T_1^*\}/N, \quad (4\cdot1)$$

where

$$\bar{T}_1 = (1/i\hbar h^6)\int d\boldsymbol{p}_2 \mathbf{S}\, \bar{g}^{(2)}(pq, rs; t)\, I(2, s) \exp[-2(\boldsymbol{p}_1-\boldsymbol{p}_p)\cdot\boldsymbol{x}_1/i\hbar]$$
$$\times \delta(\boldsymbol{p}_2-\boldsymbol{p}_q)\ \delta\Big(\boldsymbol{p}_1+\boldsymbol{p}_2-\frac{1}{2}(\boldsymbol{p}_p+\boldsymbol{p}_q+\boldsymbol{p}_r+\boldsymbol{p}_s)\Big). \quad (4\cdot2)$$

We can easily show that the time average of $g(pq, rs; t)$ defined as (3·11) becomes

$$\bar{g}^{(2)}(pq, rs; t) = \sum_{\varkappa} \{n_s(n_r - \delta_{sr})(n_q + 1 - \delta_{sq} - \delta_{rq})(n_p + 1 - \delta_{rp} - \delta_{rp} + \delta_{qp})\}^{1/2} \times \bar{\rho}^{(N)}(\varkappa; \cdots n_p + 1, n_q + 1, n_r - 1, n_s - 1 \cdots; t). \quad (4\cdot3)$$

Consequently, it is sufficient for the evaluation of the right-hand side of (4·1) to estimate the time average

$$\bar{\rho}^{(N)}(\varkappa, \varkappa'; t) = (1/\tau) \int_0^{\tau} \rho^{(N)}(\varkappa, \varkappa'; t+\nu) d\nu, \quad (4\cdot4)$$

where τ is the interval of the order of the magnitude of the mean life in collision between molecules. As we shall see later, the present calculation leads to the same result that obtained from the Born approximation for collision problems, as the result of such a choice of splitting Hamiltonian that $\Psi_{\varkappa}^{(+)} \exp(E^0(\varkappa)t/i\hbar)$, $(E^0(\varkappa) = \sum_k n_k p_i^2/2m)$, be the unperturbed wave functions for the time-dependent perturbation theory. The time-dependent perturbation theory tells us that

$$C_j(\varkappa, t+\tau) = C_j(\varkappa, t) \exp[E_{\varkappa}^0 \cdot \tau/i\hbar] - \sum_{\varkappa'} <\varkappa|U|\varkappa'> \frac{\exp[E_{\varkappa'}^0 \tau/i\hbar] - \exp[E_{\varkappa}^0 \tau/i\hbar]}{E_{\varkappa}^0 - E_{\varkappa'}^0} C_j(\varkappa', t), \quad (4\cdot5)$$

where τ is, at the longest, an interval as long as the mean life of the state corresponding to $\Psi_{\varkappa}^{(+)} \exp(E_{\varkappa}^0 t/i\hbar)$, and

$$<\varkappa|U|\varkappa'> = \int^{(N)} \cdots \int \Psi_{\varkappa}^{(+)*}(X)\, U(X)\, \Psi_{\varkappa'}^{(+)}(X)\, dX. \quad (4\cdot6)$$

Then the temporal variation of elements of the density matrix defined as (2·5) is determined by the equation

$$\rho^{(N)}(\varkappa, \varkappa'; t+\tau) = \rho^{(N)}(\varkappa, \varkappa'; t) \exp[(E_{\varkappa}^0 - E_{\varkappa'}^0)\tau/i\hbar] - \sum_{\lambda} <\varkappa|U|\lambda> \frac{\exp[(E_{\lambda}^0 - E_{\varkappa'}^0)\tau/i\hbar] - \exp[(E_{\varkappa}^0 - E_{\varkappa'}^0)\tau/i\hbar]}{E_{\varkappa}^0 - E_{\lambda}^0} \rho^{(N)}(\lambda, \varkappa'; t) - \sum_{\lambda} <\varkappa'|U|\lambda>^* \frac{\exp[(E_{\varkappa}^0 - E_{\lambda}^0)\tau/i\hbar] - \exp[(E_{\varkappa}^0 - E_{\varkappa'}^0)\tau/i\hbar]}{E_{\varkappa'}^0 - E_{\lambda}^0} \rho^{(N)}(\varkappa, \lambda; t), \quad (4\cdot7)$$

the second order infinitesimal quantities being neglected.

As suggested by Dirac[10] and Tolman[11], if we average (4·7) over all phases at the initial time t under the postulate of random *a priori* phases, non-diagonal elements of the initial density matrix all vanish, and (4·7) becomes

$$\rho^{(N)}(\varkappa, \varkappa'; t+\tau) = \rho^{(N)}(\varkappa, \varkappa; t)\, \delta_{\varkappa\varkappa'} - <\varkappa|U|\varkappa'> \frac{1 - \exp[(E_{\varkappa}^0 - E_{\varkappa'}^0)\tau/i\hbar]}{E_{\varkappa}^0 - E_{\varkappa'}^0} \{\rho^{(N)}(\varkappa', \varkappa'; t) - \rho^{(N)}(\varkappa, \varkappa; t)\}, \quad (4\cdot8)^*$$

* $\delta_{\varkappa\varkappa'} = \begin{cases} 1 & \text{if } \varkappa' \text{ is identical with } \varkappa, \\ 0 & \text{otherwise.} \end{cases}$

of which the second term contributes only to the non-diagonal elements of $\rho^{(N)}(\varkappa, \varkappa' : t+\tau)$, which give the collision term. Thus the picture of growth of the non-diagonal elements, due to the mutually non-interferent transition from every state, has been got from the assumption of random *a priori* phases at the initial time t. Then the time averaged values of non-diagonal elements of the density matrix in the N-representation are given by

$$\bar{\rho}^{(N)}(\varkappa, \varkappa' ; t) = i\hbar < \varkappa|U|\varkappa' > \{\omega(E^0_{\varkappa'} - E^0_{\varkappa})/\tau\} \{\rho^{(N)}(\varkappa, \varkappa ; t) - \rho^{(N)}(\varkappa', \varkappa' ; t)\}, \tag{4·9}$$

with

$$\omega(E^0_{\varkappa'} - E^0_{\varkappa}) = \frac{1 - \exp[(E^0_{\varkappa} - E^0_{\varkappa'})\tau/i\hbar]}{(E^0_{\varkappa} - E^0_{\varkappa'})^2} + \frac{\tau}{i\hbar(E^0_{\varkappa} - E^0_{\varkappa'})}. \tag{4·10}$$

An alternative method for deriving (4·7) will be shown in appendix.

Substitution of (4·9) into (4·3) leads to*

$$\bar{g}^{(2)} = (i\hbar/h^3) \sum_{\varkappa} \sum_{[\boldsymbol{p}_p + \boldsymbol{p}_q = \boldsymbol{p}_r + \boldsymbol{p}_s]} n_r n_s (n_p + 1)(n_q + 1) \{I(q, s) + I(q, r)\}$$
$$\times \{\omega(\epsilon_p + \epsilon_q - \epsilon_r - \epsilon_s)/\tau\} \{\rho^{(N)}(\varkappa, \varkappa ; t)$$
$$- \rho^{(N)}(\cdots, n_p + 1, n_q + 1, n_r - 1, n_s - 1, \cdots ; t)\}, \tag{4·11}$$

in which

$$\epsilon_p = P_p^2/2m. \tag{4·12}$$

Here the following relations are used:

$$< \varkappa|\sum u(i,j)|\cdots, n_p + 1, n_q + 1, n_r - 1, n_s - 1, \cdots >$$
$$= \{n_r n_s (n_p + 1)(n_q + 1)\}^{1/2} \{< rs|u|pq > + < rs|u|qp >\} \tag{4·13}$$

and

$$< rs|u|pq > = h^{-3} I(q, s)\ \delta(\boldsymbol{p}_p + \boldsymbol{p}_q - \boldsymbol{p}_r - \boldsymbol{p}_s), \tag{4·14}$$

the terms except for $p \fallingdotseq q \fallingdotseq r \fallingdotseq s$ being omitted because of the energy-momentum conservation. Inserting (4·11) in (4·2), one obtains

$$\bar{T}_1 = h^{-9} \sum_{\varkappa} \int d\boldsymbol{p}_2 \sum_{r\ [\boldsymbol{p}_1 + \boldsymbol{p}_2 = \boldsymbol{p}_r + \boldsymbol{p}_s]} \{n_r n_s (n_1 + 1)(n_2 + 1) - n_1 n_2 (n_r + 1)(n_s + 1)\}$$
$$\times \{I(2, s) + I(2, r)\}^2 \{\omega(\epsilon_1 + \epsilon_2 - \epsilon_r - \epsilon_s)/\tau\}\ \rho^{(N)}(\varkappa, \varkappa ; t). \tag{4·15}$$

Then, (4·1) becomes

$$\partial \bar{f}^{(1)}/\partial t + (\boldsymbol{p}_1/m) \cdot \nabla_{x_1} \bar{f}^{(1)} + \theta_1^{(e)} \bar{f}^{(1)}$$
$$= (h^{-9}/N) \sum_{\varkappa} \int d\boldsymbol{p}_2 \sum_{r\ [\boldsymbol{p}_1 + \boldsymbol{p}_2 = \boldsymbol{p}_r + \boldsymbol{p}_s]} \{n_r n_s (n_1 + 1)(n_2 + 1) - n_1 n_2 (n_r + 1)(n_s + 1)\}$$
$$\times \{I(2, s) + I(2, r)\}^2 \{\omega(\epsilon_1 + \epsilon_2 - \epsilon_r - \epsilon_s)/\tau\} \rho^{(N)}(\varkappa, \varkappa ; t), \tag{4·16}$$

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* Stationary external fields do not contribute to the collision term because of the energy-momentum conservation.

where

$$\Omega(x)=\omega(x)+\omega^*(x)=(\tau/\hbar)^2\sin^2(x\tau/2\hbar)/(x\tau/2\hbar)^2, \tag{4·17}$$

$\omega(x)$ being defined by (4·10).

Let us introduce the new variables

$$\boldsymbol{p}_1^0=\boldsymbol{p}_1-\boldsymbol{p},\quad \boldsymbol{p}_2^0=\boldsymbol{p}_2-\boldsymbol{p},\quad \boldsymbol{p}_r^0=\boldsymbol{p}_r-\boldsymbol{p},\quad \boldsymbol{p}_s^0=\boldsymbol{p}_s-\boldsymbol{p},$$

$$\boldsymbol{p}=\frac{1}{2}(\boldsymbol{p}_1+\boldsymbol{p}_2)=\frac{1}{2}(\boldsymbol{p}_r+\boldsymbol{p}_s). \tag{4·18}$$

And, then, the right-hand side of (4·16) is rewritten as

$$(h^{-9}/N)\sum_{\varkappa}\int d\boldsymbol{p}_2\int d\omega\{(n_rn_s(n_1+1)(n_2+1)-n_1n_2(n_r+1)(n_s+1)\}$$
$$[\boldsymbol{p}=\text{const.},\quad p_r^0=p_2^0]$$
$$\times\{I(2,r)+I(2,s)\}^2(1/\tau)\int_0^\infty p_r^{02}dp_r^0\,\Omega((p_2^{02}-p_r^{02})/m)\,\rho^{(N)}(x,x;t), \tag{4·19}$$

where $d\omega$ is the element of solid angle of deflection after collision. From the δ-function character of Ω, we have

$$\int_0^\infty p_r^{02}dp_r^0\,\Omega((p_2^{02}-p_r^{02})/m)=(m\pi/4\hbar)\,|\boldsymbol{p}_1-\boldsymbol{p}_2|\tau. \tag{4·20}$$

Hence (4·14) is expressible in the form

$$\partial\bar{f}^{(1)}/\partial t+(\boldsymbol{p}_1/m)\cdot\nabla_{x_1}\bar{f}^{(1)}+\theta_1^{(e)}\bar{f}^{(1)}$$
$$=(h^{-9}/N)\sum_{\varkappa}\int d\boldsymbol{p}_2\int d\omega\{n_rn_s(n_1+1)(n_2+1)-n_1n_2(n_r+1)(n_s+1)\}$$
$$\times a(|\boldsymbol{p}_1-\boldsymbol{p}_2|,\theta)\;\rho^{(N)}(x,x;t), \tag{4·21}$$

where $a(|\boldsymbol{p}_1-\boldsymbol{p}_2|,\theta)$ is the scattering intensity given by

$$a(p,\theta)=(m\pi/4\hbar)\left\{I\left(p\sin\frac{1}{2}\theta\right)+I\left(p\cos\frac{1}{2}\theta\right)\right\}^2p. \tag{4·22}$$

§ 5. The Boltzmann-Uehling-Uhlenbeck equation

Analogously to $g^{(2)}(pq,rs)$ defined as (3·11), we may introduce $g^{(1)}(p,r)=a_p^*a_r$, of which the diagonal elements are, as with (4·3), given by

$$g^{(1)}(\boldsymbol{p}_r,t)=\sum_{\varkappa}n_r\,\rho^{(N)}(x,x;t). \tag{5·1}$$

On the other hand, (5·1) is the expression for the momentum distribution function which may be given by

$$g^{(1)}(\boldsymbol{p},t)=N\int d\boldsymbol{x}\;f^{(1)}(\boldsymbol{x},\boldsymbol{p},t), \tag{5·2}$$

of which the reciprocal relation is given by

$$f^{(1)}(\boldsymbol{x}, \boldsymbol{p}, t) = (h^{-3}/N) \int d\boldsymbol{p}' \, e^{\boldsymbol{x}\cdot\boldsymbol{p}'/i\hbar} \, g^{(1)}\left(\boldsymbol{p}+\frac{1}{2}\boldsymbol{p}', \boldsymbol{p}+\frac{1}{2}\boldsymbol{p}' ; t\right). \tag{5·3}$$

For the system in thermal equilibrium, we shall introduce a canonical ensemble. Then, if the interactions between particles are sufficiently weak, and if no external forces act upon particles, the density matrix given by (2·5) becomes

$$\rho_0^{(N)}(\boldsymbol{x}, \boldsymbol{x}' ; t) = \{Z(T)\}^{-1} \exp\left[-E_\varkappa^0/kT\right] \delta_{\varkappa\varkappa'}, \tag{5·4}$$

where $Z(T)$ is the sum-over-states given by $\sum_\varkappa \exp(-E_\varkappa^0/kT)$. $g^{(1)}(\boldsymbol{p}, t)$ for the system in thermal equilibrium is given by

$$g_0^{(1)}(\boldsymbol{p}_r) = \sum_\varkappa n_r \{Z(T)\}^{-1} \exp\left[-E_\varkappa^0/kT\right], \tag{5·5}$$

which is independent on time. It will be easily seen from (5·5) that these $g^{(1)}(\boldsymbol{p}, t)$'s satisfy the following relations

$$g_0^{(1)}(\boldsymbol{p}_r) \, g_0^{(1)}(\boldsymbol{p}_s) = \sum_\varkappa n_r n_s \{Z(T)\}^{-1} \exp\left[-E_\varkappa^0/kT\right], \tag{5·6}$$

$$g_0^{(1)}(\boldsymbol{p}_r) \, g_0^{(1)}(\boldsymbol{p}_s) \, g_0^{(1)}(\boldsymbol{p}_t) \, g_0^{(1)}(\boldsymbol{p}_u) = \sum_\varkappa n_r n_s n_t n_u \{Z(T)\}^{-1} \exp\left[-E_\varkappa^0/kT\right], \tag{5·7}$$

if $r \neq s \neq t \neq u$. (5·6) and (5·7) show the principle of molecular chaos in quantum statistics. For the distribution slightly departing from statistical equilibrium, the similar condition may be fulfilled in the limit of vanishing density :

$$g^{(1)}(\boldsymbol{p}_r, t) \, g^{(1)}(\boldsymbol{p}_s, t) = \sum_\varkappa n_r n_s \rho^{(N)}(\boldsymbol{x}, \boldsymbol{x} ; t), \tag{5·8}$$

$$g^{(1)}(\boldsymbol{p}_r, t) \, g^{(1)}(\boldsymbol{p}_s, t) \, g^{(1)}(\boldsymbol{p}_t, t) \, g^{(1)}(\boldsymbol{p}_u, t) = \sum_\varkappa n_r n_s n_t n_u \, \rho^{(N)}(\boldsymbol{x}, \boldsymbol{x} ; t). \tag{5·9}$$

And even if the initial distribution is arbitrary, the conditions (5·8) and (5·9) may be fulfilled after an interval of time comparable to the mean life of unperturbed quantum states, so that it is expected that the time averaged functions for the distributions departing only slightly from thermal equilibrium fulfill the relation

$$\bar{g}^{(1)}(\boldsymbol{p}_r, t) \, \bar{g}^{(1)}(\boldsymbol{p}_s, t) \{\bar{g}^{(1)}(\boldsymbol{p}_t, t)+1\} \{\bar{g}^{(1)}(\boldsymbol{p}_u, t)+1\} = \sum_\varkappa n_r n_s (n_t+1)(n_u+1) \, \rho^{(N)}(\boldsymbol{x}, \boldsymbol{x} ; t). \tag{5·10}$$

This may be hold even in the presence of the external field. Time averaging both sides of (4·21) over such an interval that the relation (5·10) may be fulfilled and substitution of (5·10) into thus obtained equation give

$$\partial \bar{f}^{(1)}/\partial t + (\boldsymbol{p}_1/m) \cdot \nabla_{\boldsymbol{x}_1} \bar{f}^{(1)} + \theta_1^{(e)} \bar{f}^{(1)} = (h^{-6}/N) \int d\boldsymbol{p}_2 \int d\omega \{\bar{g}_r^{(1)} \bar{g}_s^{(s)} (\bar{g}_1^{(1)}+1)(\bar{g}_2^{(1)}+1) - \bar{g}_1^{(1)} \bar{g}_2^{(1)} (\bar{g}_r^{(1)}+1)(\bar{g}_s^{(1)}+1)\} \times a(|\boldsymbol{p}_1-\boldsymbol{p}_2|, \theta). \tag{5·11}$$

$$\left[\begin{matrix}\boldsymbol{p}_1+\boldsymbol{p}_2=\boldsymbol{p}_r+\boldsymbol{p}_s \\ \boldsymbol{p}_1^2+\boldsymbol{p}_2^2=\boldsymbol{p}_r^2+\boldsymbol{p}_s^2\end{matrix}\right].$$

If the external field is uniform, integrating (3·12) with respect to $\boldsymbol{x}$ and performing the averaging procedure as mentioned above, one obtains

$$\partial\bar{g}_2^{(1)}/\partial t+\boldsymbol{F}\cdot\nabla_{\boldsymbol{p}_1}\bar{g}_1^{(1)}$$
$$=h^{-6}\int d\boldsymbol{p}_2\int d\omega\{\bar{g}_r^{(1)}\bar{g}_s^{(1)}(\bar{g}_1^{(1)}+1)(\bar{g}_2^{(1)}+1)-\bar{g}_1^{(1)}\bar{g}_2^{(1)}(\bar{g}_r^{(1)}+1)(\bar{g}_s^{(1)}+1)\}\alpha(|\boldsymbol{p}_1-\boldsymbol{p}_2|,\theta)\cdot\left[\begin{matrix}\boldsymbol{p}_1+\boldsymbol{p}_2=\boldsymbol{p}_r+\boldsymbol{p}_s\\ \boldsymbol{p}_1^2+\boldsymbol{p}_2^2=\boldsymbol{p}_r^2+\boldsymbol{p}_s^2\end{matrix}\right] \tag{5·12}$$

As far as plane waves are used as the orthonormal set, the dependence of the phase-space d.f. $f^{(1)}$ on the spatial coordinates furnished only from the non-diagonal elements of the density matrix in the N-representation. Then, the right-hand side of (5·11) would become independent on the coordinates since the postulate of random *a priori* phases has been adopted.

On the other hand, for quantum theory of transport phenomena, Uehling and Uhlenbeck have modified the Boltzmann integro-differential equation in the following way :

$$\partial f_1/\partial t+(\boldsymbol{p}_1/m)\cdot\nabla_{\boldsymbol{x}_1}f_1-\nabla_{\boldsymbol{x}_1}u^{(e)}(\boldsymbol{x}_1)\cdot\nabla_{\boldsymbol{p}_1}f_1$$
$$=h^{-3}\int d\boldsymbol{p}_2\int d\omega\{f_rf_s(1\pm h^3f_1)(1\pm h^3f_2)-f_1f_2(1\pm h^3f_r)(1\pm h^3f_s)\}\alpha(|\boldsymbol{p}_1-\boldsymbol{p}_2|,\theta), \tag{5·13}$$

upon which most of the recent investigations on transport in quantum fluids have been based[12) 13) 14)]. Here $f_1(\boldsymbol{x},\boldsymbol{p})$ is the molecular d.f. in the phase-space and is normalized to N.

Using the postulate of random *a priori* phases in the expression (5·3), we may obtain $Nf^{(1)}=h^{-3}g^{(1)}(\boldsymbol{p},t)$. Then, if we could introduce $Nh^3f^{(1)}$ instead of $g^{(1)}$ in the right-hand side of (5·11), we would obtain the one replaced $-\nabla_{\boldsymbol{x}_1}u^{(e)}(\boldsymbol{x}_1)\cdot\nabla_{\boldsymbol{p}_1}$ in (5·13) by $\theta_1^{(e)}$. But this procedure may be validated only when $f^{(1)}$ is uniform with respect to $\boldsymbol{x}$, and approximately valid when it is nearly constant in the range of the order of the magnitude of the de Broglie wave length.

It is easily seen from the definition of $\theta_1^{(e)}$, (3·8), that the deviation from the Uehling-Uhlenbeck equation does appear under non-uniform external fields. This implies that in the Uehling-Uhlenbeck equation, (5·13), diffraction effect in the streaming terms are ignored. Uehling and Uhlenbeck arrived at the conclusion that the streaming terms are unaffected by the diffraction effect, from Kikuchi and Nordheim's theory[15)] on the kinetic fundamental equation in quantum statistics. Kikuchi and Nordheim's proof is, however, not general, because the external fields are tacitly assumed to be uniform as in Bloch's theory on the interaction between phonons and electrons, so that the conclusion of the present paper contradicts with Kikuchi and Nordheim's result in no way. It may be, however, seen from (3·8) and (5·11) that the deviation in the streaming terms due to diffraction effect is not important, if the local variations of external fields in the range of the order of the magnitude of the de Broglie wave length are not appreciable. And another kind of deviation from the Uehling-Uhlenbeck equation will be expected when $f^{(1)}$

changes with the coordinates appreciably in the range comparable to the de Broglie wave length. This may have effect on the collision term on the right-hand side of (5·13) as well as on the streaming term on the left-hand side. Thus one may expect that the integro-differential equation (5·13) is approximately valid only if both the potential energy and the phase-space d.f. change sufficiently slowly with the coordinates. While the correction due to the non-uniformity of the external fields may be given by replacing $-\nabla_{x_1} u^{(e)}(x_1)\cdot\nabla_{p_1}$ in (5·13) by $\theta_1^{(e)}$, it seems to be difficult to give the correction due to the effect of non-uniformity of the d.f. $\bar{f}^{(1)}$, since the "exact" equation for $\bar{f}^{(1)}$, (5·11), is derived only for the case where $\bar{f}^{(1)}$ is uniform with respect to the coordinates. And this uniformity results from the postulate of random *a priori* phases which has played an essential role in the derivation of (5·11).

From the above-mentioned it seems that the deviation from the Uehling-Uhlenbeck equation becomes important at such low temperatures that the de Broglie wave length is not so small compared with the dimension of the container, as in the degenerate Bose-Einstein gases, in which the wave length can be twice the linear dimension of the vessel. And it is probable that the Uehling-Uhlenbeck equation becomes invalid below the λ point and consequently the quantum-statistical interpretation of superfluidity in liquid helium II based on (5·13) might be impossible.

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Appendix

Remarks on time averaging of the N-representation of the density operator

We wish to show that the time average given in § 4 is secured from the general treatment of temporal behavior of ensemble of quantum mechanical systems, which would be valid over a long as well as a short interval of time. Let us first consider the eigenfunctions of the Hamiltonian including the perturbation due to the external fields and the molecular interactions. And let $\xi_l(q^N)$ be energy-eigenfunction belonging to the energy-eigenvalue E_l. Then one may write as follows:

$$\Phi_j(q^N, t+\tau)=\sum_l a_{jl}^0 \xi_l(q^N) \exp\left[E_l\tau/i\hbar\right], \tag{A1}$$

where

$$a_{jl}^0=\int \xi_l^*(q^N)\ \Phi_j(q^N, t)\ dq^N. \tag{A2}$$

And let us define the functions $S_l\{n_t\}$ by

$$\xi_l(q^N)=\sum_{\substack{\{n_t\}\\ [\sum n_t=N]}} S_l\{n_t\}\ \Psi^{(\pm)}_{\{n_t\}}(q^N). \tag{A3}$$

(A1) and (A3) give

$$\Phi_j(q^N, t+\tau)=\sum_{\substack{\{n_l\}\\ [\sum n_l=N]}}\sum_l a_{jl}^0 S_l\{n_l\}\ \Psi^{(\pm)}_{\{n_l\}}(q^N)\ \exp[E_l\tau/i\hbar]. \tag{A4}$$

Comparing (2·4) with (A4), one obtains

$$C_j(x, t+\tau)=\sum_l a_{jl}^0 S_l(x)\ \exp[E_l\tau/i\hbar]. \tag{A5}$$

Since the transformation given by (A3) is unitary, we have

$$\sum_\kappa S_l^*(x)\ S_m(x)=\delta_{lm}. \tag{A6}$$

Then one obtains, from (A5) and (A6),

$$a_{jl}^0=\sum_\kappa S_l^*(x)\ C_j(x, t). \tag{A7}$$

According to (A5) and (A7), the dependence of $\rho^{(N)}(x, x'; t)$ defined as (2·5) on time is given by

$$\rho^{(N)}(x, x'; t+\tau)=\sum_{x_0}\sum_{x_0'} K(x, x'|x_0, x_0':\tau)\ \rho^{(N)}(x_0, x_0':t), \tag{A8}$$

where

$$K(x, x'|x_0, x_0':\tau)=K^*(x_0, x_0'|x, x':\tau)$$
$$=\sum_l\sum_{l'} S_l(x)\ S_l^*(x_0)\ S_{l'}^*(x')\ S_{l'}(x_0')\ \exp[(E_l-E_{l'})\tau/i\hbar]. \tag{A9}$$

(A8) and (A9) correspond to Moyal's transformation equation[5] for finite interval.

Now let us consider the potential energy due to external field and the interaction between particles as the perturbation which causes the change in the energy-levels of the system. And if we make the perturbing potential tend to zero, each of the symmetrized eigenfunctions becomes identical with one of $\Psi^{(\pm)}(q^N)$'s given by (2·3). This correspondence is not necessarily one to one, unless the unperturbed energy-eigenvalues are all non-degenerate. In order to avoid unnecessary complication, non-degeneracy of the unperturbed energy-eigenvalues is assumed for the present, as in the ordinary theory of time-dependent perturbation theory, of which the result is utilized in § 4. Under this assumption $\xi_l(q^N)$ which tends to $\Psi_\kappa^{(\pm)}(q^N)$ in the limit may be expressed as $\xi_\kappa(q^N)$.

If the perturbing potential is sufficiently weak, the linear transformation given by (A3) becomes, as pointed out by Pauli[17], an infinitesimal unitary transformation represented by the matrix whose elements are

$$S_{\kappa\lambda}=\delta_{\kappa\lambda}+ib_{\kappa\lambda} \tag{A10}$$

with

$$b_{\kappa\lambda}=i\frac{\langle\lambda|U|\kappa\rangle}{E_\lambda^0-E_\kappa^0}, \tag{A11}$$

where E_κ^0 is an eigenvalue of the unperturbed Hamiltonian, and $\langle\lambda|U|\kappa\rangle$ is given by (4·6). It should be noted that the above result is nothing but an alternative formulation of the stationary perturbation theory.

Inserting (A10) in (A9) and retaining only up to the first order quantities, one obtains

$$K(\varkappa, \varkappa'|\varkappa_0, \varkappa_0' : \tau)=\delta_{\varkappa\varkappa_0}\,\delta_{\varkappa'\varkappa_0'}\exp\left[(E_\varkappa-E_{\varkappa'})\tau/i\hbar\right]$$
$$+i\,\delta_{\varkappa'\varkappa_0'}\{b_{\varkappa_0\varkappa}\exp\left[(E_{\varkappa_0}-E_{\varkappa'})\tau/i\hbar\right]+b_{\varkappa\varkappa_0}\exp\left[(E_\varkappa-E_{\varkappa'})\tau/i\hbar\right]\}$$
$$+i\,\delta_{\varkappa\varkappa_0}\{b_{\varkappa_0'\varkappa'}\exp\left[(E_\varkappa-E_{\varkappa_0'})\tau/i\hbar\right]+b_{\varkappa'\varkappa_0'}\exp\left[(E_\varkappa-E_{\varkappa'})\tau/i\hbar\right]\}. \qquad \text{(A12)}$$

From (A8) and (A12) one has

$$\rho^{(N)}(\varkappa, \varkappa' ; t+\tau)=\rho^{(N)}(\varkappa, \varkappa' ; t)\exp\left[(E_\varkappa-E_{\varkappa'})\tau/i\hbar\right]$$
$$+i\sum_{\varkappa_0}\{b_{\varkappa_0\varkappa}\exp\left[(E_{\varkappa_0}-E_{\varkappa'})\tau/i\hbar\right]+b^*_{\varkappa\varkappa_0}\exp\left[(E_\varkappa-E_{\varkappa'})\tau/i\hbar\right]\}\rho^{(N)}(\varkappa_0, \varkappa' ; t)$$
$$+i\sum_{\varkappa_0'}\{b^*_{\varkappa_0'\varkappa'}\exp\left[(E_\varkappa-E_{\varkappa_0'})\tau/i\hbar\right]+b_{\varkappa'\varkappa_0'}\exp\left[(E_\varkappa-E_{\varkappa'})\tau/i\hbar\right]\}\rho^{(N)}(\varkappa, \varkappa_0' ; t). \qquad \text{(A13)}$$

Substitution of (A11) into (A13) leads to

$$\rho^{(N)}(\varkappa, \varkappa' ; t+\tau)=\rho^{(N)}(\varkappa, \varkappa' ; t)\exp\left[(E_\varkappa-E_{\varkappa'})\tau/i\hbar\right]$$
$$-\sum_\lambda\langle\varkappa|U|\lambda\rangle\frac{\exp\left[(E_\lambda-E_{\varkappa'})\tau/i\hbar\right]-\exp\left[(E_\varkappa-E_{\varkappa'})\tau/i\hbar\right]}{E^0_\varkappa-E^0_\lambda}\rho^{(N)}(\lambda, \varkappa' ; t)$$
$$-\sum_\lambda\langle\varkappa'|U|\lambda\rangle^*\frac{\exp\left[(E_\varkappa-E_\lambda)\tau/i\hbar\right]-\exp\left[(E_\varkappa-E_{\varkappa'})\tau/i\hbar\right]}{E^0_{\varkappa'}-E^0_\lambda}\rho^{(N)}(\varkappa, \lambda ; t). \qquad \text{(A14)}$$

If one replaces $E_\varkappa$ in (A14) by the unperturbed energy-eigenvalue, $E^0_\varkappa$, this equation agrees with (5·2). This replacement would be permitted if

$$\tau\lesssim\tau_0=\hbar/(E_\varkappa-E_{\varkappa_0}). \qquad \text{(A15)}$$

From the above-mentioned, it is seen that (4·5) may be valid for the interval of the order of the magnitude of the mean life, while (A15) holds over a long as well as a short interval of time, if the perturbing potential is so weak that the series appearing in the stationary perturbation theory converges.

In the exactly analogous manner, one may obtain the change in $C_j(\varkappa, t)$ defined by (2·4) with time. Introducing (A7) into (A5) and using (A6), one has

$$C_j(\varkappa, t+\tau)=\sum_i\sum_{\varkappa'}S_i^*(\varkappa')\,S_i(\varkappa)\,C_j(\varkappa', t)\exp\left[E_i\tau/i\hbar\right]. \qquad \text{(A16)}$$

Substitution of (A10) and (A11) into (A16) leads to

$$C_j(\varkappa, t+\tau)=C_j(\varkappa, t)\exp\left[E_\varkappa\tau/i\hbar\right]$$
$$-\sum_{\varkappa'}\langle\varkappa|U|\varkappa'\rangle\frac{\exp\left[E_{\varkappa'}\tau/i\hbar\right]-\exp\left[E_\varkappa\tau/i\hbar\right]}{E^0_\varkappa-E^0_{\varkappa'}}C_j(\varkappa', t), \qquad \text{(A17)}$$

which obviously agrees with (4·5) for the interval τ not so long compared with τ_0 given by (A15). Thus the results of the time-dependent perturbation theory are obtainable from the present method.

References

1) E. A. Uehling and G. E. Uhlenbeck, Phys. Rev. **43** (1933), 552.
2) J. H. Irving and R. W. Zwanzig, J. Chem. Phys. **19** (1951), 1173.
3) E. Wigner, Phys. Rev. **40** (1932), 794.
4) J. G. Kirkwood, J. Chem. Phys. **14** (1946), 180; **15** (1947), 72.
5) J. v. Neumann, *Mathematische Grundlage der Quantenmechanik* (Berlin, 1932), Chapter 4.
6) V. Fock, ZS. f. Phys. **75** (1932), 622.
7) K. Husimi and T. Nishiyama, Prog. Theor. Phys. **5** (1950), 919.
8) J. E. Moyal, Proc. Camb. Phil. Soc. **45** (1949), 99.
9) H. Cramér, *Random Variables* (Cambridge, 1937), Second part.
10) P. A. M. Dirac, *Principles of Quantum Mechanics*, 2nd ed. (Oxford, 1935), Chapter 8.
11) R. C. Tolman, *Principles of Statistical Mechanics* (Oxford, 1938), Chapter 11.
12) A. Ishihara, J. Phys. Soc. Japan **5** (1950), 223.
13) S. Nakajima, Prog. Theor. Phys. **6** (1951), 980.
14) J. de Boer and R. B. Bird, *University of Wisconsin Nerval Research Lavoratory Reports*, No. 1509, September, 1951.
15) S. Kikuchi and L. Nordheim, ZS. f. Phys. **60** (1930), 652.
16) F. Bloch, ZS. f. Phys. **52** (1928), 555.
17) W. Pauli, *Handbuch der Physik* (Berlin, 1933), XXIV/1, p. 83.

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Effects of Tensor Forces on the Neutron-Deuteron Scattering*

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The elastic neutron-deuteron scattering cross section at 90 Mev is calculated, using the Born approximation. For neutron-neutron and neutron-proton interactions we adopt the potentials which give good agreement with nucleon-nucleon scattering experiments at high energies. Hulthén wave function is used as the ground state wave function of deuteron. The results are in better agreement with experiments than the calculations which do not take into account the tensor forces.

§ 1. Introduction

Chew[1] has first pointed out that the neutron-deuteron elastic scattering cross section was not a sum of free neutron-neutron and neutron-proton cross sections, but the interference term between them was appreciable at all energies. He also found the important fact that the ratio of elastic to total neutron-deuteron scattering cross section did not decrease so much even at rather high energies. Similar results were obtained by Hoffmann[2]. By using the sum rule, Gluckstern and Bethe[3] showed that the Born approximation in neutron-deuteron total cross section was a good approximation and got the knowledge about neutron-neutron interaction potential by comparing the experimental and theoretical neutron-deuteron total and elastic cross sections. Recently Chew[4]-[6] has formulated the so-called "impulse approximation" and applied to neutron-deuteron and proton-deuteron scattering. He found that, in the neutron-deuteron inelastic cross section, interference term between neutron-neutron and neutron-proton scattering was small and described the neutron-deuteron cross section by free two nucleon collisions and compared his results with experiments. The authors above mentioned calculated their cross sections on the assumption that the nuclear forces were central and did not consider the tensor forces.

On the other hand, Christian and Hart[7], Christian and Noyes[8], and others[9] succeeded in interpreting the experimental data on neutron-proton and proton-proton scattering by the phenomenological potential which involve tensor forces and found that the tensor forces had great effect to the angular distribution of scattered nucleons at high energies.

The purpose of the present paper is to investigate how the tensor forces affect the

* A brief account of this subject has already been published in a note in Prog. Theor. Phys **6** (1951), 623. Slight algebraic and numerical errors in the note are corrected in the present paper.

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neutron-deuteron scattering at high energies. We calculate the neutron-deuteron elastic scattering cross section, by the Born approximation, for incident energy of 90 Mev, adopting as neutron-neutron and neutron-proton potentials the ones which are given by Chamberlain et al[9]. and as the deuteron ground state wave function the so-called Hulthén wave function.

A few years ago, Wu and Ashkin[10] already gave the formulae for neutron-deuteron scattering when tensor forces were taken into account, and recently Bransden[11] performed numerical calculation following the formulation of Wu and Ashkin. However, they used Gauss functions for the radial dependence of neutron-neutron and neutron-proton potentials, as well as of deuteron ground state wave function. We will later compare their results with ours.

In § 2 we will give general formulae of neutron-deuteron elastic scattering and in § 3 the evaluation of the cross section will be given using explicit form of potentials and deuteron wave function. The results will be compared with experiments and theoretical results of other authors in § 4. In appendix, brief discussion on neutron-deuteron inelastic scattering will be developed.

§ 2. The elastic cross section

In this section, we will restrict our calculations only to the cross section of elastic scattering under the assumption that the ground state of deuteron is pure S-state. The calculation is similar to that of Gluckstern and Bethe[3], but we take also the effect of tensor forces into consideration.

Let $\boldsymbol{r}_1$, $\boldsymbol{r}_2$, and $\boldsymbol{r}_3$ be the coordinates of the neutron and proton in the deuteron and incident neutron, respectively. Then the interactions which contribute to the scattering are those between two neutrons V_{nn} and neutron-proton V_{np}. We shall choose a linear combination of Wigner, Majorana, Bartlett, and Heisenberg forces for the neutron-proton interactinn. For the neutron-neutron interactions only the Wigner and Majorana forces are necessary*.

$$V_{np}^{23} = V_{np}(r_{23})(w_p + m_p P_{23} + b_p Q_{23} + h_p P_{23} Q_{23}) + U_{np}(r_{23}) S_{23}(W_p + M_p P_{23} + B_p Q_{23} + H_p P_{23} Q_{23}) \quad (1a)$$

$$V_{nn}^{13} = V_{nn}(r_{13})(w_n + m_n P_{13}) + U_{nn}(r_{13}) S_{13}(W_n + M_n P_{13}), \quad (1b)$$

where P and Q are exchange operators with respect to the space and spin coordinates, respectively. S's are the usual tensor operators and $U(r)$'s are introduced in order to distinguish the radial dependence of the tensor forces from that of the central interactions.

The spin state of the three nucleon system consists of eight linearly independent and orthogonal states. The four of them are quartet states corresponding to a total spin 3/2. The other four are states of total spin 1/2, and we can choose two of them symmetric

* These parameters for tensor forces are not independent as can be seen directly, by observing that tensor forces vanish for the singlet state. But we include all these, so as that the formulae for tensor terms are written in parallel with that for central terms.

and the other antisymmetric in the two particles 1 and 2 in the deuteron. The quartet spin functions are designated by $\chi_i (i=1,2,3,4)$ and the doublet spin functions symmetric with respect to the two particles 1 and 2, by χ_5 and χ_6, and the ones antisymmetric, by χ_7 and χ_8. The last two are not included in the initial and final states so far as we restrict our calculations only to the elastic scattering cross section.

Then the differential cross section of the elastic scattering is given, using the Born approximation, by

$$\sigma(\theta, \phi)\, d\Omega = \frac{M^2}{9\pi^2\hbar^4}\, d\Omega\, \frac{1}{6}\sum_{i,f=1}^{6} |L^3 \mathfrak{M}_{fi}|^2, \tag{2}$$

where L^3 is a normalizing volume and $\mathfrak{M}_{fi}$ are the matrix elements

$$\mathfrak{M}_{fi} = \frac{1}{2}(\{1-P_{13}Q_{13}\}\Psi_f\chi_f, \{1-P_{13}Q_{13}\}\{V^{13}_{nn}+V^{23}_{np}\}\Psi_i\chi_i), \tag{3}$$

or by the hermitian properties of P_{13} and Q_{13}.

$$\mathfrak{M}_{fi} = (\Psi_f\chi_f, \{1-P_{13}Q_{13}\}\{V^{13}_{nn}+V^{23}_{np}\}\Psi_i\chi_i). \tag{4}$$

Ψ_i, Ψ_f and χ_i, χ_f are the initial and final space and spin wave functions and, since we are employing the Born approximation, they are given by

$$\begin{aligned} \Psi_i &= L^{-3/2} \exp\,(i\boldsymbol{k}\cdot\boldsymbol{x})\ \psi_0(r), \\ \Psi_f &= L^{-3/2} \exp\,(i\boldsymbol{k}'\cdot\boldsymbol{x})\ \psi_0(r), \end{aligned} \tag{5}$$

where $\boldsymbol{k}$ and $\boldsymbol{k}'$ are initial and final relative wave numbers between neutron and deuteron, respectively. $\boldsymbol{x}=\boldsymbol{r}_3-\frac{1}{2}(\boldsymbol{r}_1+\boldsymbol{r}_2)$ is the relative coordinate between neutron and deuteron, and $\boldsymbol{r}=\boldsymbol{r}_1-\boldsymbol{r}_2$ is the one between neutron and proton in the deuteron. $\psi_0(r)$ is the S state deuteron ground state wave function.

If we put the expression (1) for V_{nn} and V_{np} into $\mathfrak{M}_{fi}$ given in (4), and use the initial Ψ_i and final state Ψ_f given in (5), we obtain

Table I.

l	a_l	b_l	c_l
1	w_n-m_n	$w_n+\frac{1}{2}m_n$	$\frac{\sqrt{3}}{2}m_n$
2	$-w_n+m_n$	$\frac{1}{2}w_n+m_n$	$\frac{\sqrt{3}}{2}m_n$
3	w_p+b_p	$w_p-\frac{1}{2}b_p$	$\frac{\sqrt{3}}{2}b_p$
4	m_p+h_p	$m_p-\frac{1}{2}h_p$	$\frac{\sqrt{3}}{2}h_p$
5	$-w_p-b_p$	$\frac{1}{2}w_p+\frac{1}{2}b_p$	$\frac{\sqrt{3}}{2}(w_p+b_p)$
6	$-m_p-h_p$	$\frac{1}{2}m_p+\frac{1}{2}h_p$	$\frac{\sqrt{3}}{2}(m_p-h_p)$

$$L^3\mathfrak{M}_{fi}=\sum_{l=1}^{6}a_lI_l\delta_{fi}+\sum_{l=1}^{6}A_l(f|J_l|i) \quad \text{(for initial state quartet)} \tag{6a}$$

and

$$L^3\mathfrak{M}_{fi}=\sum_{l=1}^{6}b_lI_l\delta_{fi}+\sum_{l=1}^{6}B_l(f|J_l|i)+\sum_{l=1}^{6}C_l(f|J_l|i') \quad \text{(for initial state doublet)} \tag{6b}$$

where the coefficients a_l, b_l, and c_l given in table I. A_l, B_l and C_l can be obtained by replacing the small letters w, m, b, and h by W, M, B, and H. In the last term of (6b), i' should be taken as states 7 or 8 when i is 5 or 6, respectively. This term is obtained because for the doublet symmetric state, the spin exchange operators Q give a mixture χ_5 and χ_7, and the non-diagonal matrix element in spin state does not vanish in the case of tensor interaction.

J_l are given as follows:

$$J_1=\int\exp(-i\boldsymbol{k}'\cdot\boldsymbol{x})\psi_0(r)U_{nn}(|\boldsymbol{x}-\frac{1}{2}\boldsymbol{r}|)S_{13}\exp(i\boldsymbol{k}'\cdot\boldsymbol{x})\psi_0(r)d\boldsymbol{x}d\boldsymbol{r}, \tag{7a}$$

$$J_2=\int\exp(-i\boldsymbol{k}'\cdot\boldsymbol{x})\psi_0(r)U_{nn}(|\boldsymbol{x}-\frac{1}{2}\boldsymbol{r}|)S_{13}\exp[i\boldsymbol{k}(-\frac{1}{2}\boldsymbol{x}+\frac{3}{4}\boldsymbol{r})]\psi_0(|\boldsymbol{x}+\frac{1}{2}\boldsymbol{r}|)d\boldsymbol{x}d\boldsymbol{r}, \tag{7b}$$

$$J_3=\int\exp(-i\boldsymbol{k}'\cdot\boldsymbol{x})\psi_0(r)U_{np}(|\boldsymbol{x}+\frac{1}{2}\boldsymbol{r}|)S_{23}\exp(i\boldsymbol{k}\cdot\boldsymbol{x})\psi_0(r)d\boldsymbol{x}\,k\boldsymbol{r}, \tag{7c}$$

$$J_4=\int\exp(-i\boldsymbol{k}'\cdot\boldsymbol{x})\psi_0(r)U_{np}(|\boldsymbol{x}+\frac{1}{2}\boldsymbol{r}|)S_{23}\exp[-i\boldsymbol{k}(\frac{1}{2}\boldsymbol{x}+\frac{3}{4}\boldsymbol{r})]\psi_0(|\boldsymbol{x}-\frac{1}{2}\boldsymbol{r}|)d\boldsymbol{x}\,d\boldsymbol{r}, \tag{7d}$$

$$J_5=\int\exp(-i\boldsymbol{k}'\cdot\boldsymbol{x})\psi_0(r)U_{np}(r)S_{12}\exp[i\boldsymbol{k}(-\frac{1}{2}\boldsymbol{x}+\frac{3}{4}\boldsymbol{r})]\psi_0(|\boldsymbol{x}+\frac{1}{2}\boldsymbol{r}|)d\boldsymbol{x}\,d\boldsymbol{r}, \tag{7e}$$

$$J_6=\int\exp(-i\boldsymbol{k}'\cdot\boldsymbol{x})\psi_0(r)U_{np}(r)S_{12}\exp[-i\boldsymbol{k}(\frac{1}{2}\boldsymbol{x}+\frac{3}{4}\boldsymbol{r})\psi_0(|\boldsymbol{x}+\frac{1}{2}\boldsymbol{r}|)d\boldsymbol{x}\,d\boldsymbol{r}, \tag{7f}$$

and I_l are obtained form J_l by dropping the tensor operator S.

It is convenient for the treatment of J_l, to decompose $S_{ij}=3\dfrac{(\boldsymbol{\sigma}_i\boldsymbol{r}_{ij})(\boldsymbol{\sigma}_j\boldsymbol{r}_{ij})}{r_{ij}^2}-(\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j)$ into a sum of the products of two second order irreducible tensors which consist of spin operator and coordinate, respectively.

$$S_{ij}=\sum_{\mu=-2}^{2}(-1)^{\mu}Z_{-\mu}(\boldsymbol{\sigma}_i,\boldsymbol{\sigma}_j)\;Y_{2\mu}(\boldsymbol{r}_{ij}), \tag{8}$$

where

$$Z_{\pm2}=\sqrt{\frac{3}{2}}\;\sigma_i^{\pm}\,\sigma_j^{\pm}, \qquad Y_{2\pm2}=\frac{1}{2}\sqrt{\frac{3}{2}}\sin^2\theta_i\,e^{\pm2i\varphi},$$

$$Z_{\pm 1}=\mp\sqrt{\frac{3}{2}}(\sigma_{i,z}\sigma_j^{\pm}+\sigma_i^{\pm}\sigma_{j,z}), \qquad (9) \qquad Y_{2\pm 1}=\mp\sqrt{\frac{3}{2}}\sin\theta\cos\theta\, e^{\pm i\phi}, \qquad (10)$$

$$Z_0=3\sigma_{i,z}\sigma_{j,z}-(\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j), \qquad Y_{20}=\frac{1}{2}(3\cos^2\theta-1),$$

where θ and ϕ are the polar and azimuthal angles, respectively, of the direction of the relative coordinate between the particles i and j with respect to the axis of quantization. Then $(f|J_l|i)$ is written as

$$(f|J_l|i)=\sum_{\mu=-2}^{2}(-1)^{\mu}(\chi_f|Z_{-\mu}(l)|\chi_i)J_{l\mu}, \qquad (11)$$

where $J_{l\mu}$ is obtained by replacing S_{ij} in J_l by $Y_{2\mu}(\boldsymbol{r}_{ij})$. The calculation of the matrix element of $Z_\mu(l)$ is simplified by using Racah's method of tensor operator[12]. Employing his notations, we write

$$\begin{aligned}(\chi_f|Z_\mu(l)|\chi_i)&=(\alpha SM|Z_\mu(l)|\alpha' S'M')\\&=(-1)^{S+M}(\alpha S\|Z(l)\|\alpha' S')\,V(SS'2\,;-MM'\mu),\end{aligned} \qquad (12)$$

where α is introduced to descriminate the two doublet states, S is the total spin, and M is the z-component of S. These all refer to the final states, and the ones with dash correspond to initial states. The matrix elements $(\alpha S\|Z(l)\|\alpha' S')$ are given in Table II. In this table 3/2, 1/2, and 1/2′ indicate the quartet, symmetric doublet, and antisymmetric doublet states.

Table II

$(\alpha S\|Z(13)\|\alpha' S')$

S \ S'	3/2	1/2	1/2′
3/2	$4\sqrt{5}$	$-2\sqrt{5}$	$-2\sqrt{15}$
1/2	$2\sqrt{5}$	0	0
1/2′	$2\sqrt{5}$	0	0

$(\alpha S\|Z(23)\|\alpha' S')$

S \ S'	3/2	1/2	1/2′
3/2	$4\sqrt{5}$	$-2\sqrt{5}$	$2\sqrt{15}$
1/2	$2\sqrt{5}$	0	0
1/2′	$-2\sqrt{15}$	0	0

$(\alpha S\|Z(12)\|\alpha' S')$

S \ S'	3/2	1/2	1/2′
3/2	$4\sqrt{5}$	$-4\sqrt{5}$	0
1/2	$4\sqrt{5}$	0	0
1/2′	0	0	0

Substituting (6a) into (2), we obtain as the differential cross section for the initial quartet states

$$\frac{M^2}{9\pi^2\hbar^4}d\Omega\;\frac{1}{6}\sum_{i=1}^{4}\sum_{f=1}^{6}|L^3(f|\mathfrak{M}|i)|^2=\frac{M^2}{9\pi^2\hbar^4}d\Omega\left[\frac{2}{3}|\sum_l a_l I_l|^2+\frac{1}{6}\sum_{i=1}^{4}\Big(\sum_{f=1}^{4}+\sum_{f=5}^{6}\Big)|\sum_l A_l(f|J_l|i)|^2\right]. \qquad (13)$$

The second terms in the bracket is calculated applying the orthogonality relation of V's.

$$\sum_{i=1}^{4}\sum_{f=1}^{4}|\sum_l A_l\sum_\mu(-)^\mu(f|Z_{-\mu}(l)|i)J_{l\mu}|^2$$

$$=\sum_{M,M'}|\sum_{l\mu}(-)^{\mu}A_l J_{l\mu}(-)^{\frac{3}{2}+M'}\left(\frac{3}{2}\|Z(l)\|\frac{3}{2}\right)V\left(\frac{3}{2}\ \frac{3}{2}2;-M'\ M-\mu\right)|^2 \quad (14)$$

$$=\sum_{ll'}A_l A_{l'}\left(\sum_{\mu}J^*_{l\mu}J_{l'\mu}\right)\left(\frac{3}{2}\|Z(l)\|\frac{3}{2}\right)\left(\frac{3}{2}\|Z(l')\|\frac{3}{2}\right)\cdot\frac{1}{5}$$

$$=\sum_{ll'}A_l A_{l'}\frac{(4\sqrt{5})^2}{5}\sum_{\mu}J^*_{l\mu}J_{l'\mu}=16\sum_{\mu}|\sum_{l}A_l J_{l\mu}|^2.$$

In a similar way we get for the third term

$$4\sum_{\mu}|\sum_{l=1}^{4}A_l J_{l\mu}-2\sum_{l=5}^{6}A_l J_{l\mu}|^2. \quad (15)$$

Thus, (13) becomes as

$$\frac{M^2}{9\pi^2\hbar^4}d\Omega\left\{\frac{2}{3}|\sum_{l}a_l I_l|^2+\frac{8}{3}\sum_{\mu}|\sum_{l}A_l J_{l\mu}|^2+\frac{2}{3}\sum_{\mu}|\sum_{l=1}^{4}A_l J_{l\mu}-2\sum_{l=5}^{6}A_l J_{l\mu}|^2\right\}. \quad (16)$$

The calculation for initial doublet states is similar as for initial quartet states, and we get, summing them

$$\sigma(\theta,\phi)d\Omega=\frac{M^2}{9\pi^2\hbar^4}d\Omega\ \frac{1}{6}\left[\frac{2}{3}|\sum_{l}a_l I_l|^2+\frac{8}{3}\sum_{\mu}|\sum_{l}A_l J_{l\mu}|^2+\frac{2}{3}\sum_{\mu}|\sum_{l=1}^{4}A_l J_{l\mu}-2\sum_{l=5}^{6}A_l J_{l\mu}|^2\right.$$

$$\left.+\frac{1}{3}|\sum_{l}b_l I_l|^2+\frac{2}{3}\sum_{\mu}|\sum_{l=1}^{4}(B_l-\sqrt{3}C_l)J_{l\mu}-2\sum_{l=5}^{6}B_l J_{l\mu}|^2\right]. \quad (17)$$

The total cross section σ is obtained by integrating over solid angle. We decompose σ, for later convenience, into the sum of the contributions from neutron-proton and neutron-neutron interactions and their interference. We write them as σ_{np}, σ_{nn}, and σ_{int}, respectively. They are

$$\sigma_{np}=\frac{M^2}{9\pi^2\hbar^4}\ \frac{1}{6}\int d\Omega\left[\frac{2}{3}|\sum_{l=3}^{6}a_l I_l|^2+\frac{8}{3}\sum_{\mu}|\sum_{l=3}^{6}A_l J_{l\mu}|^2+\frac{2}{3}|\sum_{l=3}^{4}A_l J_{l\mu}-2\sum_{l=5}^{6}A_l J_{l\mu}|^2\right.$$

$$\left.+\frac{1}{3}|\sum_{l=3}^{6}b_l I_l|^2+\frac{2}{3}\sum_{\mu}|\sum_{l=3}^{6}(B_l-\sqrt{3}C_l)J_{l\mu}-2\sum_{l=5}^{6}B_l J_{l\mu}|^2\right],$$

$$\sigma_{nn}=\frac{M^2}{9\pi^2\hbar^4}\ \frac{1}{6}\int d\Omega\left[\frac{2}{3}|\sum_{l=1}^{2}a_l I_l|^2+\frac{8}{3}\sum_{\mu}|\sum_{l-1}^{2}A_l J_{l\mu}|^2+\frac{2}{3}|\sum_{l=1}^{2}A_l J_{l\mu}|^2\right.$$

$$\left.+\frac{1}{3}|\sum_{l=1}^{2}b_l I_l|^2+\frac{2}{3}\sum_{\mu}|\sum_{l=1}^{2}(B_l-\sqrt{3}C_l)J_{l\mu}|^2\right], \quad (18)$$

$$\sigma_{int}=\frac{M^2}{9\pi^2\hbar^4}\ \frac{1}{6}\int d\Omega\left[\frac{2}{3}(\sum_{l=3}^{6}a_l I_l)^*(\sum_{l=1}^{2}a_l I_l)+\frac{8}{3}\sum_{\mu}(\sum_{l=3}^{6}A_l J_{l\mu})^*(\sum_{l=1}^{2}A_l J_{l\mu})\right.$$

$$\left.+\frac{2}{3}\sum_{\mu}(\sum_{l=3}^{4}A_l J_{l\mu}-2\sum_{l=5}^{6}A_l J_{l\mu})^*\sum_{l=1}^{2}A_l J_{l\mu}+\frac{1}{3}(\sum_{l=3}^{6}b_l I_l)^*(\sum_{l=1}^{2}b_l I_l)\right.$$

$$+\frac{2}{3}\sum_{\mu}\Big(\sum_{l=3}^{6}(B_l-\sqrt{3}\,C_l)J_{l\mu}-2\sum_{l=5}^{6}B_lJ_{l\mu}\Big)^*\Big(\sum_{l=1}^{2}(B_l-\sqrt{3}\,C_l)J_{l\mu}\Big)$$

$$+comp.\ conj.].$$

§ 3. The evaluation of the cross section

In evaluating the integral I_l and $J_{l\mu}$ we intruduce following Fourier transform of potentials and deuteron wave function

$$V(q)=\int V(r)\exp(\pm i\boldsymbol{q}\cdot\boldsymbol{r})\,d\boldsymbol{r}, \tag{19a}$$

$$U_\mu(\boldsymbol{q})=\int U(r)\,Y_{2\mu}(\boldsymbol{r})\,\exp(\pm i\boldsymbol{q}\cdot\boldsymbol{r})\,d\boldsymbol{r}, \tag{19b}$$

$$\psi_0(q)=\int\psi_0(r)\exp(\pm i\boldsymbol{q}\cdot\boldsymbol{r})\,d\boldsymbol{r}, \tag{20a}$$

$$\psi_0^2(q)=\int\psi_0(r)^2\exp(\pm i\boldsymbol{q}\cdot\boldsymbol{r})\,d\boldsymbol{r}, \tag{20b}$$

and put $\boldsymbol{x}-\frac{1}{2}\boldsymbol{r}=\boldsymbol{\xi}$, $\boldsymbol{k}'-\boldsymbol{k}=\boldsymbol{q}$. Then we obtain;

$$I_1=V_{nn}(q)\psi_0^2\Big(\frac{q}{2}\Big), \tag{21a}$$

$$I_2=(2\pi)^{-3/2}\int d\boldsymbol{p}\psi_0(p)\psi_0(|\tfrac{1}{2}\boldsymbol{q}+\boldsymbol{p}|)\,V_{nn}(|\tfrac{1}{2}\boldsymbol{k}+\boldsymbol{k}'+\boldsymbol{p}|), \tag{21b}$$

$$I_3=V_{np}(q)\psi_0^2\Big(\frac{q}{2}\Big), \tag{21c}$$

$$I_4=(2\pi)^{-3/2}\int d\boldsymbol{p}\psi_0(p)\psi_0(|\tfrac{1}{2}\boldsymbol{q}+\boldsymbol{p}|)\,V_{np}(|\tfrac{1}{2}\boldsymbol{k}+\boldsymbol{k}'+\boldsymbol{p}|), \tag{21d}$$

$$I_5=I_6=\psi_0(|\tfrac{1}{2}\boldsymbol{k}+\boldsymbol{k}'|)\int d\boldsymbol{r}\psi_0(r)\,V_{np}(r)\exp[i\tfrac{1}{2}(\boldsymbol{k}+\tfrac{1}{2}\boldsymbol{k}')\cdot\boldsymbol{r}]. \tag{21e}$$

$$J_{1\mu}=U_{nn,\mu}(\boldsymbol{q})\psi_0^2(q/2), \tag{22a}$$

$$J_{2\mu}=(2\pi)^{-3/2}\int d\boldsymbol{p}\psi_0(p)\psi_0(|\tfrac{1}{2}\boldsymbol{p}+\boldsymbol{q}|)U_{nn,\mu}(\tfrac{1}{2}\boldsymbol{k}+\boldsymbol{k}'+\boldsymbol{p}), \tag{22b}$$

$$J_{3\mu}=U_{np,\mu}(\boldsymbol{q})\psi_0^2(q/2), \tag{22c}$$

$$J_{4\mu}=(2\pi)^{-3/2}\int d\boldsymbol{p}\psi_0(p)\psi_0(|\tfrac{1}{2}\boldsymbol{p}+\boldsymbol{q}|)U_{nn,\mu}(\tfrac{1}{2}\boldsymbol{k}+\boldsymbol{k}'+\boldsymbol{p}), \tag{22d}$$

$$J_{5\mu}=J_{6\mu}=\psi_0(|\tfrac{1}{2}\boldsymbol{k}+\boldsymbol{k}'|)\int d\boldsymbol{r}\psi_0(r)\,U_{np}(r)\,Y_{2\mu}(\boldsymbol{r})\exp[i\tfrac{1}{2}(\boldsymbol{k}+\tfrac{1}{2}\boldsymbol{k}')\boldsymbol{r}]. \tag{22e}$$

We have obtained our results, thus far, without the use of an explicit potential. However, we must now choose a particular form for the potential and for the deuteron ground state wave function. We shall use for the potential the ones which Chamberlain

et al.[9] showed to fit well for neutron-proton and proton-proton scattering at high energies. On the assumption of charge independence we use proton-proton potential for neutron-neutron potential. They are ;

$$V_{np}^{23}=\begin{cases}(-35.3\text{Mev})\,(1/2+1/2P_{23})\varphi_1(r), & \text{for singlet state}\\ (-25.3\text{Mev})\,(1/2+1/2P_{23})\varphi_1(r)+(-48.2\text{Mev})\,(0.37+0.63P_{23})\varphi_1(r)S_{23}, & \text{for triplet state}\end{cases} \tag{23}$$

$$V_{nn}^{13}=\begin{cases}(-13.27\text{Mev})\,(1/2+1/2P_{13})\varphi_2(r) & \text{for singlet state}\\ (-15.25\text{Mev})\varphi_3(r)S_{13} & \text{for triplet state}\end{cases} \tag{24}$$

where

$$\varphi_1(r)=(\lambda_1 r)^{-1}e^{-\lambda_1 r} \qquad 1/\lambda_1=1.35\times10^{-13}\text{cm}, \tag{25a}$$

$$\varphi_2(r)=\begin{cases}1 & r<r_2\\ 0 & r>r_2\end{cases} \qquad r_2=2.615\times10^{-13}\text{cm}, \tag{25b}$$

$$\varphi_3(r)=(\lambda_3 r)^{-2}e^{-\lambda_3 r} \qquad 1/\lambda_3=1.6\times10^{-13}\text{cm}. \tag{25c}$$

Then the numerical values of w etc. are given as follows :

$$w_p=-15.1\text{Mev}, \quad W_p+B_p=-17.8\text{Mev}, \quad w_n=-6.7\text{Mev}, \quad W_n-M_n=-15.25\text{Mev}.$$
$$m_p=-15.1\text{Mev}, \quad M_p+H_p=-30.4\text{Mev} \quad m_n=-6.7\text{Mev}, \tag{26}$$
$$b_p=2.5\text{Mev},$$
$$h_p=2.5\text{Mev}.$$

Here we obtain the explicit form of (19):

$$V_{nn}(q)=\int\varphi_2(r)\exp(\pm i\boldsymbol{q}\cdot\boldsymbol{r})d\boldsymbol{r}=4\pi r_2^3\{\sin(qr_2)-(qr_2)\cos(qr_2)\}/(qr_2)^2, \tag{27a}$$

$$U_{nn,\mu}(\boldsymbol{q})=\int\varphi_3(r)Y_{2\mu}(\boldsymbol{r})\exp(\pm i\boldsymbol{q}\cdot\boldsymbol{r})d\boldsymbol{r}$$
$$=4\pi Y_{2\mu}(\boldsymbol{q})\left\{\frac{1}{2}\left(1+3\frac{\lambda_3^2}{q^2}\right)\tan^{-1}\frac{q}{\lambda_3}-\frac{3\lambda_3}{q}\right\}/\lambda_3 q, \tag{27b}$$

$$V_{np}(q)=\int\varphi_1(r)\exp(\pm i\boldsymbol{q}\boldsymbol{r})d\boldsymbol{r}=4\pi/\lambda_1(\lambda_1^2+q^2), \tag{27c}$$

$$U_{np,\mu}(\boldsymbol{q})=\int\varphi_1(r)\exp(\pm i\boldsymbol{q}\boldsymbol{r})Y_{2\mu}(\boldsymbol{r})d\boldsymbol{r}$$
$$=4\pi Y_{2\mu}(\boldsymbol{q})\left[1+\frac{3}{2}\frac{\lambda_1^2}{q^2}\left\{1-\left(\frac{q}{\lambda_1}+\frac{\lambda_1}{q}\right)\tan^{-1}\frac{q}{\lambda_1}\right\}\right]/\lambda_1(q^2+\lambda_1^2), \tag{27d}$$

For deuteron ground state wave function we use the Hulthén wave function :

$$\psi_0(r)=N\frac{e^{-\alpha r}-e^{-\beta r}}{r}, \quad N^2=\frac{\alpha\beta(\alpha+\beta)}{2\pi(\alpha-\beta)^2}, \tag{28}$$

where $\alpha=0.213\times10^{13}\text{cm}^{-1}$, $\beta=1.638\times10^{13}\text{cm}^{-1}$, and the Fourier transform of $\psi_0(r)$

and $\psi_0(r)^2$ are :

$$\psi_0(q)=\int\psi_0(r)\exp(\pm i\boldsymbol{q}\cdot\boldsymbol{r})\,d\boldsymbol{r}=4\pi N\Big(\frac{1}{\alpha^2+q^2}-\frac{1}{\beta^2+q^2}\Big), \tag{29a}$$

$$\psi_0^2(q)=\int\psi_0(r)^2\exp(\pm i\boldsymbol{q}\cdot\boldsymbol{r})\,d\boldsymbol{r}=\pi N^2\Big(\tan^{-1}\frac{q}{2\alpha}-\tan^{-1}\frac{q}{\alpha+\beta}+\tan^{-1}\frac{q}{2\beta}\Big)/q \tag{29b}$$

The Fourier transform of $\psi_0(r)\,l^{-}_{np}(r)$ and $\psi_0(r)U_{nn}(r)Y_{2\mu}(\boldsymbol{r})$ in (21a) and (22e) are similarly calculated. We put them into (23) and (24) and the results are

$$I_1=(4\pi)^2r_2^3\frac{2N^2}{q}\,\frac{\sin qr_2-qr_2\cos qr_2}{(qr_2)^2}\Big\{\tan^{-1}\frac{q}{4\alpha}-\tan^{-1}\frac{q}{2(\alpha+\beta)}+\tan^{-1}\frac{q}{4\beta}\Big\}, \tag{30a}$$

$$I_2=\frac{(4\pi)^2}{(2\pi)^{3/2}}\int d\boldsymbol{p}\,N^2\Big(\frac{1}{\alpha^2+p^2}-\frac{1}{\beta^2+p^2}\Big)\Big(\frac{1}{\alpha^2+|\tfrac{1}{2}\boldsymbol{q}+\boldsymbol{p}|^2}-\frac{1}{\beta^2+|\tfrac{1}{2}\boldsymbol{q}+\boldsymbol{p}|^2}\Big)r_2^2$$
$$\times\frac{\sin(|\boldsymbol{z}+\boldsymbol{p}|r_2)-(|\boldsymbol{z}+\boldsymbol{p}|r_2)\cos(|\boldsymbol{z}+\boldsymbol{p}|r_2)}{(|\boldsymbol{z}+\boldsymbol{p}|r_2)^2}, \tag{30b}$$

$$I_3=(4\pi)^2\frac{1}{\lambda_1(\lambda_1^2+q^2)}\,\frac{2N^2}{q}\Big\{\tan^{-1}\frac{q}{4\alpha}-\tan^{-1}\frac{q}{2(\alpha+\beta)}+\tan^{-1}\frac{q}{4\beta}\Big\}, \tag{30c}$$

$$I_4=\frac{(4\pi)^2}{(2\pi)^{3/2}}\int d\boldsymbol{p}N^2\Big(\frac{1}{\alpha^2+p^2}-\frac{1}{\beta^2+p^2}\Big)\Big(\frac{1}{\alpha^2+|\tfrac{1}{2}\boldsymbol{q}+\boldsymbol{p}|^2}-\frac{1}{\beta^2+|\tfrac{1}{2}\boldsymbol{q}+\boldsymbol{p}|^2}\Big) \tag{30d}$$
$$\times\frac{1}{\lambda_1(\lambda_1^2+|\boldsymbol{z}+\boldsymbol{p}|^2)},$$

$$I_5=I_6=(4\pi)^2N^2\Big(\frac{1}{\alpha^2+z^2}-\frac{1}{\beta^2+z^2}\Big)\frac{1}{\mu_1 z}\Big(\tan^{-1}\frac{z}{\alpha+\mu_1}-\tan^{-1}\frac{z}{\beta+\mu_1}\Big), \tag{30e}$$

$$J_{1\mu}=(4\pi)^2\frac{Y_{2\mu}(\boldsymbol{q})}{\lambda_3 q}\Big\{\frac{1}{2}\Big(1+3\frac{\lambda_3^2}{q^2}\Big)\tan^{-1}\frac{q}{\lambda_3}-\frac{3\lambda_3}{q}\Big\}\frac{2N^2}{q}$$
$$\times\Big\{\tan^{-1}\frac{q}{4\alpha}-\tan^{-1}\frac{q}{2(\alpha+\beta)}+\tan^{-1}\frac{q}{4\beta}\Big\}, \tag{31a}$$

$$J_{2\mu}=\frac{(4\pi)^2}{(2\pi)^{3/2}}\int d\boldsymbol{p}N^2\Big(\frac{1}{\alpha^2+p^2}-\frac{1}{\beta^2+p^2}\Big)\Big(\frac{1}{\alpha^2+|\tfrac{1}{2}\boldsymbol{q}+\boldsymbol{p}|^2}-\frac{1}{\beta^2+|\tfrac{1}{2}\boldsymbol{q}+\boldsymbol{p}|^2}\Big)\frac{Y_{2\mu}(\boldsymbol{z}+\boldsymbol{p})}{\lambda_3^2|\boldsymbol{z}+\boldsymbol{p}|}$$
$$\times\Big\{\frac{1}{2}\Big(1+3\frac{\lambda_3^2}{|\boldsymbol{z}+\boldsymbol{p}|^2}\Big)\tan^{-1}\frac{|\boldsymbol{z}+\boldsymbol{p}|}{\lambda_3}-3\frac{\lambda_3}{|\boldsymbol{z}+\boldsymbol{p}|}\Big\}, \tag{31b}$$

$$J_{3\mu}=(4\pi)^2\frac{Y_{2\mu}(q)}{\lambda_1(q^2+\lambda_1^2)}\Big[1+\frac{3}{2}\frac{\lambda_1^2}{q^2}\Big\{1-\Big(\frac{q}{\lambda_1}+\frac{\lambda_1}{q}\Big)\tan^{-1}\frac{q}{\lambda_1}\Big\}\Big]\frac{2N^2}{q}$$
$$\times\Big\{\tan^{-1}\frac{q}{4\alpha}-\tan^{-1}\frac{q}{2(\alpha+\beta)}+\tan^{-1}\frac{q}{4\beta}\Big\}, \tag{31c}$$

$$J_{4\mu}=\frac{(4\pi)^2}{(2\pi)^{3/2}}\int d\boldsymbol{p}N^2\left(\frac{1}{\alpha^2+p^2}-\frac{1}{\beta^2+p^2}\right)\left(\frac{1}{\alpha^2+|\frac{1}{2}\boldsymbol{q}+\boldsymbol{p}|^2}-\frac{1}{\beta^2+|\frac{1}{2}\boldsymbol{q}+\boldsymbol{p}|^2}\right)$$
$$\times\frac{Y_{2\mu}(\boldsymbol{z}+\boldsymbol{p})}{\lambda_1(|\boldsymbol{z}+\boldsymbol{p}|^2+\lambda_1^2)}\left[1+\frac{\lambda_1^2}{|\boldsymbol{z}+\boldsymbol{p}|^2}\left\{1-\left(\frac{|\boldsymbol{z}+\boldsymbol{p}|}{\lambda_1}+\frac{\lambda_1}{|\boldsymbol{z}+\boldsymbol{p}|}\right)\tan^{-1}\frac{|\boldsymbol{z}+\boldsymbol{p}|}{\lambda_1}\right\}\right] \quad (31d)$$

$$J_{3\mu}=J_{6\mu}=(4\pi)^2N^2\left(\frac{1}{\alpha^2+z^2}-\frac{1}{\beta^2+z^2}\right)\frac{Y_{2\mu}(\boldsymbol{z}')}{\lambda_1 z}$$
$$\times\left[\frac{\beta-\alpha}{2z}+\frac{1}{2}\left\{1+3\frac{(\alpha+\lambda_1)^2}{z^2}\right\}\tan^{-1}\frac{z}{\alpha+\lambda_1}-\frac{1}{2}\left\{1+3\frac{(\beta+\lambda_1)^2}{z^2}\right\}\tan^{-1}\frac{z}{\beta+\lambda_1}\right] \quad (31e)$$

where $\boldsymbol{z}=\frac{1}{2}\boldsymbol{k}+\boldsymbol{k}'$, $\boldsymbol{z}'=\boldsymbol{k}+\frac{1}{2}\boldsymbol{k}'$.

For I_2, I_4, $J_{2\mu}$, and $J_{4\mu}$ we must further integrate, but the last integration over p can only be performed by numerical integration. These calculations are lengthy, so we do not write here.

§ 4. Calculated results and comparison with experiments

In Table III we show the total cross section of elastic scattering with tensor interaction and Stern's[13] experimental value for proton-deuteron scattering.* For comparison, the

Table III. Cross sections in mb.

	G-B Serber	Our results			Experiment
		Central part	Tensor part	Total	
σ_{np}	32	11	5	16	
σ_{nn}	16	8	9	17	
σ_{int}	23	12	−2	10	
σ_{nd}	71[a]	31	12	43	28±3[b]

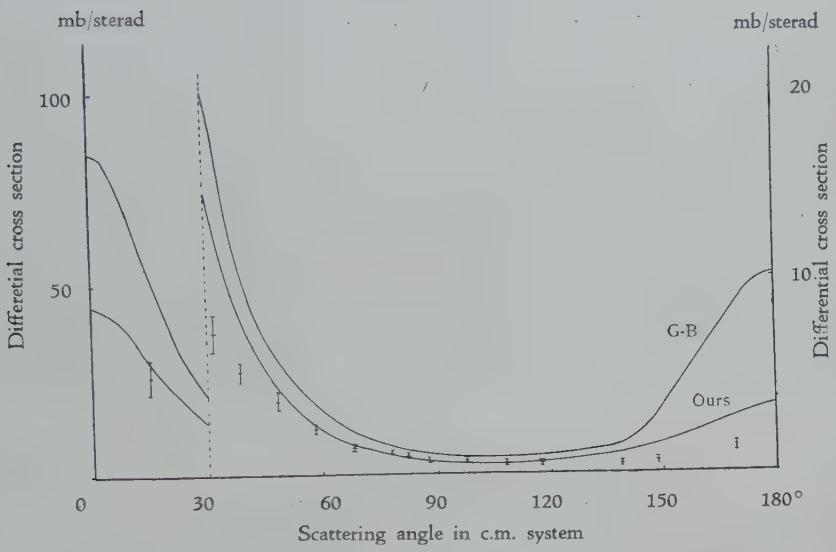
a: Gluckstern and Bethe gave 60 mb for this value.
b: In previous note we adopted Powell's data; 35mb.

one with central interaction only is shown. It is calculated by using Gluckstern and Bethe's potential which is Serber type for neutron-neutron force and is determined so as to agree with experiment for total (elastic plus inelastic) cross section. Our result is smaller and have better agreement with experiment than Gluckstern and Bethe's. The reason will be as follows: (i) the interference between neutron-neutron and neutron-proton scattering is destructive for tensor part, and (ii) when tensor forces are taken into account,

* Stern gives the elastic differential scattering cross section of 190 Mev deuterons by protons, which corresponds to the scattering of 95 Mev protons by deuterons. At high energies as 90 Mev there will appear no difference between neutron-deuteron and proton-deuteron scattering except for small angles. Therefore we can compare our calculations with his results.

Fig. 1. Differential cross section of elastic scattering

G-B Theoretical: Gluckstern and Bethe's
Ours Theoretical: Ours
I Experimental: Stern's



the contribution from the central to the cross section is reduced more than half of the value obtained without tensor forces, and the contribution from tensor potentials is too small to cover this reduction. A possible explanation of this result will be given in appendix.

The angular distribution of scattered nucleon is shown in Fig. 1. As is seen from the figure our results agree better with experiments than Gluckstern and Bethe's. Especially the backward scattering cross section is about ten times larger than the experimental value in the case of central interaction only, while our calculation is only twice larger. This will also be caused by the same reason (ii), mentioned in the discussion of the total cross section, and this effect is natually enhanced in the forward and backward scattering.

Though our results are in better agreement with experiments, the total cross section and backward scattering are yet too large compared with experiments. One reason of this result will be, that the total cross sections for high energy nucleon-nucleon collisions, which were calculated by using the same potentials, were already larger than experimental values. On the other hand, it was shown by Buckingham and Massey[14], that the result for 20 Mev neutron-deuteron scattering with the Born approximation, calculated by Verde[15], gave higher backward scattering than their result with exact calculation. Though Verde's high backward scattering might have been caused by the use of Gauss error function in his calculation, and the energy 20 Mev, in their case, was much smaller than 90 Mev, in our case, the use of the Born approximation may be considered to give another reason to interpret our high values.

The elastic total cross section of Bransden[11] is much larger than ours, and we suppose that this is because he used Gauss function for both nuclear potential and deuteron ground state wave function. However, as it is known that, though the total cross section for nucleon-nucleon collision is not sensitive to the radial dependence of potentials, the angular distribution calculated using Gauss potential is in worse agreement than the one calculated using long range potential[7], so the difference between his result and ours will appear more in the angular than in the total cross section. Bransden's result gives too small side scattering and this is clearly in disagreement with experiment.

The effect of D-state in deuteron ground state, though they are small enough to be neglected for total cross section as shown by Bransden, they may affect to reduce the angular distribution of backward scattering.

Acknowledgement

The authors wish to express their sincere thanks to Prof. T. Yamanouchi for his kind interest and to Messrs. Y. Fujimoto and Y. Yamaguchi for their helpful discussion. Two of the authors (T.T. and S.Y.) are indebted to the Yumiuri Fellowship for the financial aid.

Appendix

Results with impulse approximation

In the text we confined our calculation only to the elastic scattering. Here we will discuss the elastic and inelastic scattering i.e. total cross section. By the recipe of the impulse approximation, Chew had formulated for the neutron-deuteron scattering[4] and analyzed experimental data[5], but he has not taken into account of the non-central forces. In CII* the neutron-deuteron scattering cross section was described by the two body neutron neutron and neutron-proton cross sections, but the expression must be changed if the tensor forces are included. Though, in general, the two and three body collision cross sections cannot be separated into central and tensor force cross sections, we can do this if we use the Born approximation in accord with the approximation used in the text. We use this expedient in the following calculation.

Writing the tensor operator S_{ij}, as the scalar product of two vectors, as in (8) in the text

$$S_{ij}=\frac{3(\boldsymbol{\sigma}_i\cdot\boldsymbol{r}_{ij})(\boldsymbol{\sigma}_j\cdot\boldsymbol{r}_{ij})}{r_{ij}^2}-(\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j)=\sum_{\mu}(-)^{\mu}Y_{\mu 2}(\boldsymbol{r}_{ij})Z_{-\mu}(\boldsymbol{\sigma}_i,\boldsymbol{\sigma}_j), \qquad \text{(A-1)}$$

and defining the scattering amplitude, $R^T_{ij,\mu}$ by

$$R^T_{ij,\mu}=\left(\boldsymbol{k}_{ij}\left|Y_{2\mu}(\boldsymbol{r}_{ij})U(r_{ij})\right|\frac{\boldsymbol{k}_0+\boldsymbol{k}_1}{2}\right), \qquad \text{(A-2)}$$

the neutron-proton and neutron-neutron cross sections are given as follows**

* We refer Chew's paper (reference 5) as CII.

** We use same notation as in CII, except for tensor terms.

$$\sigma_{np}^{total}=\frac{2\pi}{\hbar v_0}\left(\frac{Mk_0}{4\hbar^2}\right)\int d\omega_{1p}\left[\frac{3}{4}|r_{1p}^{t}|^2+\frac{1}{4}|r_{1p}^{s}|^2+6\sum_{\mu}|R_{1p,\mu}^{T}|^2,\right], \tag{A-3}$$

$$\sigma_{nn}^{total}=\frac{2\pi}{\hbar v_0}\left(\frac{Mk_0}{4\hbar^2}\right)\int d\omega_{12}\left[\frac{3}{4}|r_{12}^{t}-r_{21}^{t}|^2+\frac{1}{4}|r_{12}^{s}+r_{21}^{s}|^2+6\sum_{\mu}|R_{12,\mu}^{T}-R_{21,\mu}^{T}|^2\right]. \tag{A-4}$$

The total neutron-deuteron cross section is given, after some calculation, as

$$\sigma_{nd}^{total}=\sigma_{nd}^{central}+\frac{2\pi}{\hbar v_0}\int d\boldsymbol{k}_2 g_2(\boldsymbol{k}_2)\left(\frac{Mk_{1p}}{2\hbar^2}\right)\int d\omega_{1p}\left[6\sum_{\mu}|R_{1p,\mu}^{T}|^2\right]$$

$$+\frac{2\pi}{\hbar v_0}\int d\boldsymbol{k}_p g_0(\boldsymbol{k}_p)\left(\frac{Mk_{1p}}{4\hbar^2}\right)\int d\omega_{12}\left[6\sum_{\mu}|R_{12,\mu}^{T}-R_{21,\mu}^{T}|^2+I^T-P^T\right]. \tag{A-5}$$

Here $\sigma_{nd}^{central}$ is the same expression as in CII (12); I^T is the tensor part of the interference term between neutron-proton and neutron-neutron scattering, and P^T is the tensor part of the Pauli exclusion term. Comparing with (A-3) and (A-4), and using the result of CII for the central part, we can rewrite (A-5) as follows

$$\begin{aligned}\sigma_{nd}^{total}&=(1-\epsilon^c)\sigma_{np}^{central}+\sigma_{nn}^{central}+I^c\\&\quad+(1-\epsilon^T)\sigma_{np}^{tensor}+\sigma_{nn}^{tensor}+I^T.\end{aligned} \tag{A-6}$$

I^c is the central part of the interference term and it is given in Table III in the text together with I^T. ϵ^c and ϵ^T is to be determined by comparing the angular distribution of high energy protons with experiment. But it is found, in the approximation similar to deriving (22) of CII, that the tensor terms contribute nothing to the forward scattering, so we can put $\epsilon^T=0$, and it is also permitted to put ϵ^c equal to ϵ of CII, i.e. $\epsilon^c=0.15$.

The neutron-deuteron elastic cross section is obtained in a similar way,

$$\sigma_{nd}^{elastic}=\bar{S}(\sigma_{np}^{central}+\frac{3}{2}\sigma_{nn}^{central}+I^c+\frac{2}{3}\sigma_{np}^{tensor}+\frac{4}{3}\sigma_{nn}^{tensor}+I^T), \tag{A-7}$$

and it becomes, if we use for $\bar{S}$ the value 0.28 following CII

$$\sigma_{nd}^{elastic}=0.28\sigma_{nd}^{central}+0.42\,\sigma_{np}^{central}+I_c+0.19\sigma_{np}^{tensor}+0.37\sigma_{nn}^{tensor}+I^T. \tag{A-8}$$

To determine $\sigma_{np}^{central}$ etc., we calculate these cross sections by the Born approximation, using for potentials those used in the text, and normalize them so that the sum of the central and tensor cross sections give the experimental total neutron-proton and neutron-neutron (proton-proton) cross sections. The results are given in Table A-1.

Table A-I

$\sigma_{np}{}^{c}$	$\sigma_{np}{}^{T}$	$\sigma_{nn}{}^{c}$	$\sigma_{nn}{}^{T}$
35	38	18	17mb

Using these values, and those of I^c, I^T, ϵ^c, and ϵ^T, obtained above, we are now able to calculate the σ_{nd}^{total} and $\sigma_{nd}^{elastic}$, and obtained for them 113 mb and 41 mb, respectively. The former agrees fairly well with the experimental value 117mb given by McMillan[16], and the latter with the value 43 mb obtained in the text.

Though the 41 mb is a little larger than the experimental value of Stern, it is conceivably smaller than the value 50mb calculated by Chew in CII. The reason will clearly be seen from (A-8), in which the coefficients for tensor terms are smaller the corresponding ones for central terms, both for neutron-proton and neutron-neutron cross sections, and also from the fact that our $I^c+I^T=12.2-1.8=10.4$mb is much smaller than the value 15mb used by Chew. These considerations will perhaps clarify the fact, that the total elastic cross section obtained in the text, with inclusion of tensor forces was much smaller than the one without inclusion of them.

References

1) G. F. Chew, Phys. Rev. **74**(1948), 809.
2) F. de Hoffman, Phys. Rev. **78**(1950), 216.
3) R. L. Gluckstern and H. A. Bethe, Phys. Rev. **81**(1951), 761.
4) G. F. Chew, Phys. Rev. **80**(1950), 196.
5) G. F. Chew, Phys. Rev. **84**(1951), 710.
6) G. F. Chew, Phys. Rev. **84**(1951), 1057.
   See also, P. B. Daitch and J. B. French, Phys. Rev. **85**(1951), 695.
7) R. S. Christian and E. W. Hart, Phys. Rev. **77**(1950), 441.
8) R. S. Christian and H. P. Noyes. Rev. **79**(1951), 85.
9) O. Chamberlain, E. Segrè and C. Wiegand, Phys. Rev. **83** (1951), 923.
10) T. Y. Wu and J. Ashkin, Phys. Rev. **73**(1948), 986.
11) B. H. Bransden, Proc. Roy. Soc. **209A** (1951), 380.
12) G. Racah, Phys. Rev. **62**(1942), 438.
13) M. O. Stern, private communication.
    We are indebted to Dr. Stern for his kind information of new experimental results prior to publiction.
14) R. Buckingham, S. J. Hubbard, and H. S. W. Massey, Proc. Roy. Soc. **211A** (1952), 83.
15) M. Verde, Helv. Phys. Acta **22**(1949), 339.
16) L. J. Cook, E. M. McMillan, J. M. Peterson, and D. C. Sewell, Phys. Rev. **75**(1949), 7.

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On the Electronic Structures of the *M*-Centers in Alkali-halide Crystals.

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The electronic energy levels of the *M*-centers in the colored LiCl and NaCl crystals are calculated by LCAO method, assuming Seitz's model. The ground state and the first excited state (optically permitted) are shown to belong to A_1 and B_1 symmetry, respectively, the wave-lengths of the optical transition between them being in comparatively good agreement with the observed *M*-absorption peaks.

§ 1. Introduction

Of the various color-centers in alkali-halides, we already know much about the *F*-center,[1)2)] and recently many experimental results have been reported on the natures of the several bands which appear on the long[2)3)] and short[4)5)] wave-length sides of the *F*-absorption band.

The color-centers which correspond to these absorption bands are divided, as regards their structures, into two groups: those due to trapped *electrons*, and those due to trapped *holes*.[6)] We shall confine ourselves to the former group in the following.

By irradiation to or thermal treatments of the *F*-colored crystal, several absorption bands appear one after another, of which the most prominent and stable is the *M*-band. This band, first observed by Ottmer[7)] and investigated later by Molnar,[2)] appears together with the *F*-band in the X-ray colored crystal, or even in the additively colored crystal under suitable thermal treatments, though it is obtained most conspicuously when the *F*-colored crystal is irradiated with the *F*-absorption light.

Seitz[2)] proposed a model for the *M*-center which is responsible for the *M*-absorption band, by analysing the experimental facts on the mutual transformations between the *M*- and the other (F, R_1, R_2) absorption bands, and by presuming existence of pairs and quartets of positive and negative vacancies. This model seems to be rather plausible as it is consistent with various experimental results hitherto reported.

Recently Petroff[3)] has carried out very detailed and suggestive experiments on the formation and disintegration of various bands from the *F*-band. According to these results, the *M*-band plays an important part as an intermediate product in the formation of various bands from the *F*-band. Consequently it seems to be very important to investigate theoretically the structure of the *M*-center and its relation to those of the other centers.

In the present paper we calculate the energy levels of the M–center for the case of LiCl and NaCl with the method of LCAO, assuming Seitz's model stated above, and compare the results with experiments.

§ 2. Symmetry of the M–center and classification of electronic states

According to Seitz,[2] the M–center consists of L–shaped vacancies - *one positive* and *two negative ion vacancies* as is shown in Fig. 1 — where *an electron* is trapped, so that it is electrically neutral as a whole. As the vacancy complex is larger than the F–center, the electron trapped there will be strongly localized to this region, consequently the effect of polarization seems to decrease rapidly as one goes away from the center. Assuming the rigid lattice from this reason, as in the previous calculation on the F–center,[8] we calculate in the present paper the electronic energy levels of the M–center, using LCAO method.

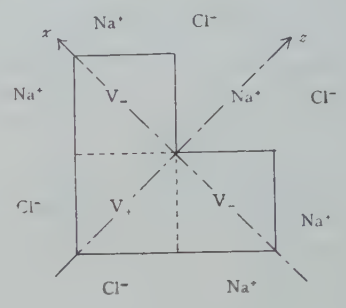

Fig. 1. Seitz's model for the M–center.

As is seen from Fig. 1, the potential for the trapped electron has a symmetry axis of order two (z–axis), and a symmetry plane of reflexion (xz–plane), so that its symmetry is C_{2v}. If the electron under consideration occupies rather shallow traps below conduction band, as is the case for the F–center, it seems to be adequate to approximate the wave function of the trapped electron with linear combination of alkali atom orbitals.

The alkali ions around the center can be classified according to symmetry as is shown in Fig. 2, the same Greek letters being assigned to the equivalent ions. The potential of C_{2v} symmetry yields four types of states — A_1, B_1, A_2, B_2, wave function of each of which should be constructed from atomic orbitals of the alkali ions in Fig. 1 with the coefficients as shown in Tab. 1, where the orbitals should be taken as $2s$ and $2p$ for Li, $3s$ and $3p$ for Na, etc.….

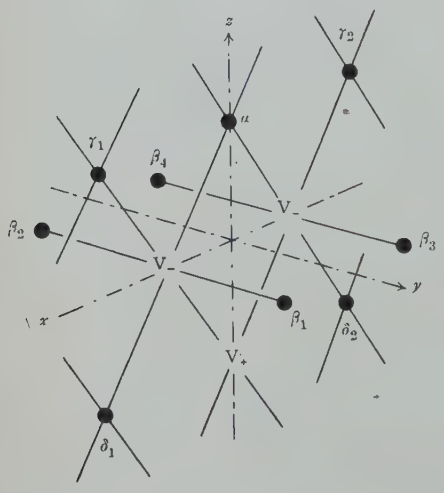

Fig. 2. Classification of alkali-ions in the immediate neighbourhood of the center.

The ground state is of course A_1 state, from which transitions are permitted to A_1, B_1 and B_2 states.

In the present calculation, we take s– and p–orbitals for the α–ion, only s–orbitals for β–ions and neglect γ– and δ–ion orbitals, as it is rather laborious to solve secular equations of higher degrees. In Tab. 1, the

Table I. The LCAO coefficients for the four classes of states

		α	β				γ		δ	
			1	2	3	4	1	2	1	2
A_1	s	1	1	1	1	1	1	1	1	1
	p_z	1	1	1	1	1	1	1	1	1
	p_x		1	1	−1	−1	1	−1	1	−1
	p_y		1	−1	1	−1				
A_2	s		1	−1	−1	1				
	p_z		1	−1	−1	1				
	p_x		1	−1	1	−1				
	p_y		1	1	−1	−1	1	−1	1	−1
B_1	s		1	1	−1	−1	1	−1	1	−1
	p_z		1	1	−1	−1	1	−1	1	−1
	p_x	1	1	1	1	1	1	1	1	1
	p_y		1	−1	−1	1				
B_2	S		1	−1	1	−1				
	p_z		1	−1	1	−1				
	p_x		1	−1	−1	1				
	p_y	1	1	1	1	1	1	1	1	1

orbitals used in the following calculation are written in Gothic type; we have to solve secular equations of the third degree for A_1 states, and of the second degree for B_1 and B_2 states.

§ 3. Calculation of energy levels

The Hamiltonian for the trapped electron is taken as

$$H=-\frac{1}{2}\Delta+\sum_{(\text{all ions})}V^i.$$

where V^i is the potential due to the i-th ion, which is fixed at its lattice point because we take here the rigid lattice model as stated above. We assign $i=0$ for the α-ion, $i=1$, 2, 3, 4 for the β-ions, and write $V^{ij\cdots k}$ to mean the potential due to all ions except the i-, j-,$\cdots$ and k-th ions.

The wave functions are written as follows:

A_1 state : $\Psi = a_1 \Phi_1 + a_2 \Phi_2 + a_3 \Phi_3$,

$$\begin{cases} \Phi_1 = \psi_{s,0} , \\ \Phi_2 = \psi_{z,0} , \\ \Phi_3 = \psi_{s,1} + \psi_{s,2} + \psi_{s,3} + \psi_{s,4} , \end{cases}$$

B_1 state : $\Psi = \beta_1 \Phi_1 + \beta_2 \Phi_2$,

$$\begin{cases} \Phi_1 = \psi_{x,0} , \\ \Phi_2 = \psi_{s,1} + \psi_{s,2} - \psi_{s,3} - \psi_{s,4} , \end{cases}$$

B_2 state : $\Psi = \gamma_1 \Phi_1 + \gamma_2 \Phi_2$,

$$\begin{cases} \Phi_1 = \psi_{y,0} , \\ \Phi_2 = \psi_{s,1} - \psi_{s,2} + \psi_{s,3} - \psi_{s,4} , \end{cases}$$

where ψ_s, ψ_z are s– and p–orbitals, the suffices which stand to the right of these signify the ion numbers to which the given atomic orbitals belong.

We have only to solve the secular equations

$$\text{Det.} \, | H_{mn} - \Delta_{mn} E | = 0 ,$$

with

$$H_{mn} = \int \Phi_m H \Phi_n \, d\tau ,$$

$$\Delta_{mn} = \int \Phi_m \Phi_n \, d\tau ,$$

for the above states.

We have calculated for the case of LiCl and NaCl ; the orbitals, numerical values, methods of approximation used are as follows.

Calculations of the matrix elements H_{mn} reduce to those of the integrals of the type such as

$$\int \psi_{s,1} H \psi_{z,0} \, d\tau ,$$

where we take advantage of the relations of atomic orbitals ;

$$\left(-\frac{1}{2} \Delta + V^i \right) \psi_{s,i} = E^s \psi_{s,i} ,$$

$$\left(-\frac{1}{2} \Delta + V^i \right) \psi_{x,i} = E^p \psi_{x,i} ,$$

E^s and E^p being, for instance, $2s$ and $2p$ levels of Li atom for the case of lithium halides. The numerical values of E^s and E^p are taken from spectro-scopic data, giving in atomic unit :

	Li	Na
E^s	−0.1981	−0.1889
E^p	−0.1302	−0.1116 .

In calculating two-center integrals of

$$\begin{cases} a\text{–type} & \int \psi_i V^j \psi_j d\tau\,, \\ b\text{–type} & \int \psi_i V^j \psi_i d\tau\,, \end{cases}$$

and three-center integrals of

$$\int \psi_i V^j \psi_k d\tau\,,$$

we have used the atomic orbitals of Slater,[9] that is:

$$\text{Li} \quad \begin{cases} \psi_s = \dfrac{N}{\sqrt{4\pi}} r \exp(-\mu r), \\ \psi_z = \dfrac{\sqrt{3}N}{\sqrt{4\pi}} r \cos\theta \exp(-\mu r), \\ \mu = 0.65\,, \end{cases}$$

$$\text{Na} \quad \begin{cases} \psi_s = \dfrac{N}{\sqrt{4\pi}} r^2 \exp(-\mu r), \\ \psi_z = \dfrac{\sqrt{3}N}{\sqrt{4\pi}} r^2 \cos\theta \exp(-\mu r), \\ \mu = 0.733\,. \end{cases}$$

As for the three-center integrals, we first take summation over the ions

$$\int \psi_i \Big(\sum_{j\neq i,k} V^j\Big) \psi_k d\tau = \int \psi_i V^{(ik)} \psi_k d\tau\,,$$

and replace the potential $V^{(ik)}$ by its value at the maximum point of $\psi_i \psi_k$, taking into account the fact that the potential is a comparatively slowly varying function in the neighbourhood of the i–th and j–th ions.

Moreover in calculating two- and three-center integrals, we approximated the potentials V^j by Coulomb potentials $\mp 1/r_j$ according as the ion is positive or negative, after ascertaining that it produces comparatively small differences in comparison with the case of approximation with Hartree potential.

When we take summations over j of the two-center integrals, those of the a–type integrals consist of finite terms, while those of the b–type integrals consist of infinite terms. For example, one of the b–type integrals is calculated as

$$\int \psi_{z,i}(\mp/r_j)\psi_{z,i} d\tau = \mp\frac{1}{R_{ij}} \mp \frac{3}{2\mu^2}\{3\cos^2(\widehat{z, R_{ij}}) - 1\}\frac{1}{R_{ij}^3}$$

$$+ \text{exponentially vanishing term},$$

for the $2p$–orbitals (that is, for Li). For s–orbitals the second term does not appear as the latter is a term due to quadripole moment of the charge distribution of p–state. Now when we take summation of these integrals over j, the sum of the first terms gives Madelung potential if the crystal is perfect, so that in this case we have only to subtract the contributions of the absent ions. The sum of the second terms should be zero for

the perfect crystal owing to cubic symmetry, so that we have to take sum only over the absent ions and then to reverse sign. In summing the third terms, only the several nearest ions will suffice, for they vanish rather rapidly as one goes away from the i–th ion.

The b–type integrals of the form such as

$$\int \psi_{s,i}(\mp 1/r_j)\psi_{z,i}d\tau$$

are calculated as

$$\cos(\widehat{z, R_{ij}})f(R_{ij}),$$

the sum of which over j is zero for perfect crystal on account of cubic symmetry, so we have only to sum over the absent ions and reverse the sign.

As regards the overlap integrals and two-center integrals we referred to the formulae in the paper of Mulliken and his collaborators.[9]

For the lattice distances we have used the following values :

$$\text{LiCl}: d=3.92, \quad \text{NaCl}: d=4.36.$$

The matrix elements are expressed in terms of the above integrals as follows :

A_1 state :

$$\Delta_{11}=1, \quad \Delta_{22}=1, \quad \Delta_{12}=0,$$

$$\Delta_{33}=4\{1+S_{s,s}(\sqrt{2}\,d)+S_{s,s}(2d)+S_{s,s}(\sqrt{6}\,d)\},$$

$$\Delta_{13}=4S_{s,s}(\sqrt{2}\,d),$$

$$\Delta_{23}=-2S_{s,p\sigma}(\sqrt{2}\,d),$$

$$H_{11}=E^s+(\psi_0^s,\ V^{(0)},\ \psi_0^s),$$

$$H_{22}=E^p+(\psi_{z,0},\ V^{(0)},\ \psi_{z,0}),$$

$$H_{33}=E^s\Delta_{33}+4\{(\psi_{s,1},\ V^{(1)},\ \psi_{s,1})+(\psi_{s,1},\ V^{(12)},\ \psi_{s,2})+(\psi_{s,1},\ V^{(13)},\ \psi_{s,3})$$
$$+(\psi_{s,1},\ V^{(14)},\ \psi_{s,4})\}+4\{U_{s,s}(\sqrt{2}\,d)+U_{s,s}(2d)+U_{s,s}(\sqrt{6}\,d)\},$$

$$H_{12}=(\psi_{z,0},\ V^{(0)},\ \psi_{s,0}),$$

$$H_{13}=E^s\Delta_{13}+4(\psi_{s,0},\ V^{(01)},\ \psi_{s,1})+4U_{s,s}(\sqrt{2}\,d),$$

$$H_{23}=E^s\Delta_{23}+4(\psi_{z,0},\ V^{(01)}\psi_{s,1})-2U_{p\sigma,s}(\sqrt{2}\,d),$$

B_1 state :

$$\Delta_{11}=1,$$

$$\Delta_{22}=4\{1-S_{s,s}(\sqrt{2}\,d)+S_{s,s}(2d)-S_{s,s}(\sqrt{6}\,d)\},$$

$$\Delta_{12}=2S_{p\sigma,s}(\sqrt{2}\,d),$$

$$H_{11}=E^p+(\psi_{x,0},\ V^{(0)},\ \psi_{x,0}),$$

$$H_{22}=E^s\Delta_{22}+4\{(\psi_{s,1},\ V^{(1)},\ \psi_{s,1})+(\psi_{s,1},\ V^{(12)},\ \psi_{s,2})-(\psi_{s,1},\ V^{(13)},\ \psi_{s,3})$$
$$-(\psi_{s,1},\ V^{(14)},\ \psi_{s,4})\}+4\{-U_{s,s}(\sqrt{2}\,d)+U_{s,s}(2d)-U_{s,s}(\sqrt{6}\,d)\},$$

$$H_{12}=E^s\Delta_{12}+4(\psi_{x,0},\ V^{(01)},\ \psi_{s,1})+2U_{p\sigma,s}(\sqrt{2}\,d),$$

B_2 state :

$$\Delta_{11}=1,$$

$$\Delta_{22}=4\{1+S_{s,s}(\sqrt{2}\,d)-S_{s,s}(2d)-S_{s,s}(\sqrt{6}\,d)\},$$

$$\Delta_{12}=2\sqrt{2}\,S_{s,p\sigma}(\sqrt{2}\,d),$$

$$H_{11}=E^p+(\psi_{y,0},\ V^{(0)},\ \psi_{y,0}),$$

$$H_{22}=E^s\Delta_{22}+4\{(\psi_{s,1},\ V^{(1)},\ \psi_{s,1})-(\psi_{s,1},\ V^{(12)},\ \psi_{s,2})+(\psi_{s,1},\ V^{(13)},\ \psi_{s,3})$$
$$-(\psi_{s,1},\ V^{(14)},\ \psi_{s,4})\}+4\{U_{s,s}(\sqrt{2}\,d)-U_{s,s}(2d)-U_{s,s}(\sqrt{6}\,d)\},$$

$$H_{12}=E^s\Delta_{12}+4(\psi_{y,0},\ V^{(01)},\ \psi_{s,1})+2\sqrt{2}\,U_{p\sigma,s}(\sqrt{2}\,d).$$

Here $S(R)$ is the overlap integral of the atomic orbitals of two ions separated by R, and U is the two-center integral ; for example,

$$\int\psi_{p\sigma,i}V^s\psi_{s,j}d\tau=U_{p\sigma,s}(R_{ij})=U_{s,p\sigma}(R_{ij}).$$

§ 4. Results of calculation and some remarks on the approximations[10]

As the procedure of calculation used here is essentially the variation method, it will give rather reliable values of energy for the lowest states of A_1, B_1, B_2, respectively, though the overlap integrals are fairly large. The results of calculation are given in Tab. 2.

Table 2. Results of calculation and comparison with experiments (in eV)

	Calculation				Observed M-absorption peaks
	A_1	B_1	B_2	$A_1\rightarrow B_1$	
LiCl	−4.86	−2.76	−1.45	2.10	1.90
NaCl	−5.63	−3.90	−1.45	1.73	1.72

The values of the energy levels of A_1 and B_1 states are, at first sight, too deep. But when the trapped electron is raised to the conduction band thermally or optically, there is left a defect with total charge $+1$, the medium polarizing radially from the center, with lowering of the crystal energy as a whole. The extent of this lowering is given as follows :

for *thermal* process : $$\frac{1}{2}\phi+\chi=\frac{1}{2}\left(1-\frac{1}{\varkappa}\right)\frac{1}{R}+\chi,$$

for *optical* transition : $$\frac{2}{2}\phi_0+\chi=\frac{1}{2}\left(1-\frac{1}{\varkappa_0}\right)\frac{1}{R}+\chi,$$

where $\varkappa$ and $\varkappa_0$ are dielectric constants at low and high frequencies, respectively, χ is the work function of the crystal, and R is the effective radius of the M-center. Thermal

and optical depths of a state are obtained by subtracting the above quantities from the values given in Tab. 2, thus leading to fairly shallow traps.

Although the absolute values of energy given in Tab. 2 have no direct physical meanings as stated above, their differences between any two states will give, on the other hand, fairly good values for optical transition, because in these trapped states the distribution of the electron differs rather in symmetry than in range, thus making plausible the assumption that the energy due to polarization is much the same in all the states. If we assume that the M–absorption band is due to the transition from A_1 state to B_1 state, the calculated wave-lengths are in good agreement with observations, as is shown in Tab. 2.

As the vacancy complex of the M–center is fairly large, the shielding effect of potential due to polarization is, perhaps, too weak in the direct neighbourhood of it to use bulk properties $\varkappa$ and $\varkappa_0$ in describing the polarization. Thus the method used here, in spite of neglection of the polarization effect, seems to be a comparatively adequate way of describing the essential aspects of the matter. If we deal, however, with the interrelations of the trapped states and the conduction band, the polarization effect will play a very important part.

§ 5. Conclusion and additional remarks

We have calculated the energy levels of the M–center, with the LCAO method, for the cases of LiCl and NaCl, assuming Seitz's model for its structure, and obtained the wave-lengths of $A_1 \rightarrow B_1$ transition in good agreement with the observed values of the M–band. The calculation given here includes, however, various approximations, so that it might yet be too early to conclude that Seitz's presumption on the structure of the M–center is confirmed by it.

After this work was announced in the Annual Meeting of the Physical Society of Japan, 1950, Ueta[11] has performed interesting experiments on the bleaching of the M–band by polarized light, and confirmed to a certain extent that Seitz's model for the M–center is plausible and that the transition perhaps takes place from A_1 to B_1, not, at least, from A_1 to B_2; in agreement with our results.

References

1) N. F. Mott and R. W. Gurney, *Electronic Processes in Ionic Crystals* (Oxford, 1940), Chapter 4.
2) F. Seitz, Rev. Mod. Phys. **18** (1946), 348.
3) S. Petroff, ZS. f. Phys. **127** (1950), 443.
4) R, Casler, P. Pringsheim and P. Yuster, Journ. Chem. Phys. **18** (1950), 887; 1564.
5) J. Alexander and E. E. Schneider, Nature **164** (1949), 653.
6) T. Inui, Y. Uemura and Y. Toyozawa, Busseiron-Kenkyu **38** (1951), 42.
7) R. Ottmer, ZS. f. Phys. **46** (1928), 798.
8) T. Inui and Y. Uemura, Prog. Theor. Phys. **5** (1950), 252.
9) R. S. Mulliken, C. A. Rieke, D. Orloff and H. Orloff, Journ. Chem. Phys. **17** (1949), 1248.
10) H. F. Ivey, Phys. Rev. **72** (1947), 341.
11) M. Ueta, Journ. Phys. Soc. Japan **7** (1952), 107.

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Selection Rules for Decays of π–Mesons and V–Particles

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Making use of the general principle of invariance under space rotation and inversion, the decay of a π–meson into two Fermions and a V–particle (assuming spin 1/2) into one Boson and one Fermion are investigated. The subject of interest is: whether any of these decay processes can be made forbidden by assigning appropriate parities to various Fermions, as has been remarked by Yang and Tiomno. It is found that there exists no such possibility, that is, there is no reasonable assignments of parities which make any processes forbidden. This result is reexamined in the light of charge independence hypothesis, in which π–meson fields are considered to interact charge symmetrically with nucleon and lepton fields. It is found, however, that the introduction of this hypothesis does not better the situation at all. Several definite conclusions are drawn on the isotopic angular momenta of V–particles from this hypothesis. Discussions are also made on the possibility of the proposed model in which μ–mesons and V–particles are assumed to be the excited states of leptons and nucleons, respectively.

§ 1. Introduction

One of us (MS)[1] has recently proposed the possibility to reduce the number of elementary particles by assuming that μ–mesons and V–particles are the excited states of leptons and nucleons, respectively. According to the idea leptons and nucleons are excited up to μ–mesons and V–particles respectively, through their interactions with π–meson fields. If one adopts this idea it is unnecessary to assume any Fermi-type interactions and one again has the possibility of explaining the β–decay processes with Yukawa's original theory.

One encounters, however, with difficulties, which were already mentioned by us[1], in adopting this idea. If μ–mesons are really the excited states of leptons one cannot exclude the experimentally almost forbidden processes[2]

$$\pi^{\pm} \rightarrow e^{\pm} + \nu ,$$

which may well take place in $\sim 10^{-8}$ sec., so that one can reasonably explain the β–decay phenomena. Similar difficulties arise for the decay of a V–particle. That is, one can never exclude the possibility of a V^0–particle decaying into a nucleon and a π–meson,

$$V^0 \rightarrow N + \pi^0,$$
$$\rightarrow P + \pi^-,$$

whereas the favorable decay mode is[3]

$$V^0 \rightarrow P + \pi^- + \pi^0,$$
$$\rightarrow N + \pi^+ + \pi^-.$$

The present work intends to meet these difficulties making use of the principle of general invariance under space rotation and inversion. The result is, however, negative for both processes as will be seen in what follows.

This method of obtaining the most general selection rules was developed by Yang[4] for the case of the dematerialization of a particle into two photons. In this paper his method is extended to investigate the decays of charged π–mesons and l–particles assuming they have spin zero and $1/2$, respectively. Some complications arise for these decay processes which did not appear in Yang's investigation. They are all due to the appearance of Fermi particles in final states.

The wave functions for spin $1/2$ particles can assume four different types specified with their transformation properties under space inversion. This point was also investigated by Yang and Tiomno[5] in connection with the possibility of assuming the universal Fermi-type interactions. In the present paper, however, we are on the different stand point from these authors', since we do not assume any Fermi-type interactions. On this point discussions are made in Section 2.

Since we deal with the processes in which the number of particles is not a constant of motion, we are obliged to use the quantized field theory to formulate the principle of invariance under space rotation and inversion. This is done by expressing various states in terms of creation operators and vacuum states as will be discussed in Section 3.

In Section 4 transformation properties of various states are discussed to obtain selection rules for decay processes. Discussions for the obtained results are made in Section 5 in the light of charge independence hypothesis for π–nucleon and π–lepton interactions. Summary of results are found in Section 6. A remark on the connection of the method of configuration space with that of second quantization, especially in case of the existence of antiparticles besides the ordinary ones, is given in Appendix.

§ 2. Preliminary considerations

In order that a particle can disintegrate into two or more final products, the initial and final states must have the same transformation properties under space rotation and inversion. This general principle of invariance makes it possible to obtain selection rules for the processes under consideration. It should be noted that the selection rules thus obtained are quite independent of the type of assumed interactions in a sense that, if a negative conclusion is drawn with this method for a certain process, it can never be allowed whatever type of interactions one may assume. On the contrary, positive conclusions cannot be valid if we do not assume any interactions which are responsible for the process. Thus we are not restricted by all of Yang and Tiomno's results[5], since we have no concern with any Fermi-type interactions.

(*a*) *Decay of π–mesons*

We are going to investigate whether the processes

$$\pi^+ \rightarrow \bar{e} + \nu \qquad (1)$$

and $$\pi^- \rightarrow e + \bar{\nu} \qquad (2)$$

can be forbidden by appropriately assigning different parities to electron and neutrino fields.

It seems, at first sight, that we can do this by assigning real parities to the electron field, while imaginary ones to the neutrino, or *vice versa*. If we do this, however, π–mesons can never interact with lepton fields, since then we can by no means construct any invariant couplings from these three fields. Thus we have four possibilities left for the final state. They are:

case (A): (e, ν) have the same real parities.
case (B): (e, ν) have the different real parities.
case (C): (e, ν) have the same imaginary parities.
case (D): (e, ν) have the different imaginary parities.*

We assume π–mesons have spin zero. As to the parities we note that this is closely related with those of nucleons. Clark, Roberts, and Wilson[6] observed that π–mesons have odd parities if the proton and neutron have the same real or different imaginary parities. If, on the contrary, the proton and neutron have the different real or same imaginary parities, π–mesons should be of even parities in contrast with the usually accepted idea. This fact will be used in discussing the decay of a V^0–particle.

Thus we have, in investigating the decay of a charged π–meson, eight possible cases in all, two for the initial and four for the final states.

(β) *Decay of V^0–particles*

Since protons and neutrons interact with π–meson fields, the case in which protons have real parities while neutrons have imaginary ones, or *vice versa*, is excluded. The process

$$V^0 \rightarrow P + \pi^- + \pi^0, \text{ or } \rightarrow N + \pi^+ + \pi^-$$

should be allowed for and hence, if nucleons have real (imaginary) parities V^0–particles must also have real (imaginary) ones, respectively. Thus in considering the process

$$V^0 \rightarrow N + \pi^0, \qquad (3)$$

or

$$V^0 \rightarrow P + \pi^-, \qquad (4)$$

we have four possibilities for the combinations of a V^0 and a nucleon just similar to those for electron-neutrino combinations given in (α). For each of them π–mesons may have even or odd parities. We have here eight possible cases specified with parities:**

	V^0	nucleon	π
case (A)′:	1	1	±1
case (B)′:	1	−1	±1
case (C)′:	i	i	±1
case (D)′:	i	$-i$	±1.

* If one considers an electron and a neutrino as the different isotopic spin states of unified leptons, the cases (B) and (D) are naturally excluded.

** One can also assume parities −1 and $-i$ for V^0–particles. We consider, however, only these eight cases, since nothing new arises if we include them.

§ 3. Representation of states

We specify π-meson and spin 1/2 fields with φ and ψ, respectively. φ is scalar or pseudoscalar, while ψ is spinor. It is assumed that $l^{\prime\prime}$-particles have spin 1/2 and neutrinos have finite mass.

Let us consider the expansion of a q-number spinor $\psi(\boldsymbol{r})$ in terms of annihilation and creation operators. We write

$$\psi(\boldsymbol{r})=\sum_{\boldsymbol{K}} u(\boldsymbol{K})e^{i\boldsymbol{K}\boldsymbol{r}}, \tag{5}$$

and put[7]

$$u(\boldsymbol{K})=(K^2+k^2)^{-(1/2)}\left\{a_{\boldsymbol{K}}^{(1)}\begin{bmatrix}K\\0\\k_3\\k_1\end{bmatrix}+a_{\boldsymbol{K}}^{(2)}\begin{bmatrix}0\\K\\k_2\\-k_3\end{bmatrix}+b_{-\boldsymbol{K}}^{(2)*}\begin{bmatrix}-k_3\\-k_1\\K\\0\end{bmatrix}+b_{-\boldsymbol{K}}^{(1)*}\begin{bmatrix}-k_2\\k_3\\0\\K\end{bmatrix}\right\}, \tag{6}$$

where $K=k_0+m$, $k_0=(m^2+k^2)^{1/2}$, $k=|\boldsymbol{K}|$, $k_1=k_x+ik_y$, $k_2=k_x-ik_y$, and $k_3=k_z$*. As is easily seen, operators a's and b's satisfy the commutation relations

$$\{a_{\boldsymbol{K}}^{(i)*},\ a_{\boldsymbol{K}'}^{(j)}\}=\{b_{\boldsymbol{K}}^{(i)*},\ b_{\boldsymbol{K}'}^{(j)}\}=\delta_{ij}\delta(\boldsymbol{K},\ \boldsymbol{K}'),\quad i,j=1,2. \tag{7}$$

$$\textit{all other anticommutators}=0,$$

corresponding to

$$\{u_m^*(\boldsymbol{K}),\ u_n(\boldsymbol{K}')\}=\delta_{mn}\delta(\boldsymbol{K},\ \boldsymbol{K}'),$$

$$\{u_m^*(\boldsymbol{K}),\ u_n^*(\boldsymbol{K}')\}=\{u_m(\boldsymbol{K}),\ u_n(\boldsymbol{K}')\}=0,\quad m,n=1,2,3,4.$$

For special $\boldsymbol{K}$ parallel to z axis (6) can be simplified to

$$u(\boldsymbol{K})=(K^2+k^2)^{-(1/2)}\left\{a_{\boldsymbol{K}}^{(1)}\begin{bmatrix}K\\0\\k\\0\end{bmatrix}+a_{\boldsymbol{K}}^{(2)}\begin{bmatrix}0\\K\\0\\-k\end{bmatrix}+b_{-\boldsymbol{K}}^{(2)*}\begin{bmatrix}-k\\0\\K\\0\end{bmatrix}+b_{-\boldsymbol{K}}^{(1)*}\begin{bmatrix}0\\k\\0\\K\end{bmatrix}\right\}. \tag{8}$$

One readily sees for this special case,

$$u^*(\boldsymbol{K})[a_z k+\beta m]u(\boldsymbol{K})=k_0({}^{(a)}N_{\boldsymbol{K}}^{(1)}+{}^{(a)}N_{\boldsymbol{K}}^{(2)}+{}^{(b)}N_{-\boldsymbol{K}}^{(2)}+{}^{(b)}N_{-\boldsymbol{K}}^{(1)}-2), \tag{9}$$

$$\int dV\, e^{-i\boldsymbol{K}\boldsymbol{r}}u^*(\boldsymbol{K})\left[\frac{1}{i}\frac{\partial}{\partial r}\right]u(\boldsymbol{K})e^{i\boldsymbol{K}\boldsymbol{r}}=\boldsymbol{K}({}^{(a)}N_{\boldsymbol{K}}^{(1)}+{}^{(a)}N_{\boldsymbol{K}}^{(2)}-{}^{(b)}N_{-\boldsymbol{K}}^{(2)}-{}^{(b)}N_{-\boldsymbol{K}}^{(1)}+2), \tag{10}$$

$$u^*(\boldsymbol{K})\sigma_z u(\boldsymbol{K})={}^{(a)}N_{\boldsymbol{K}}^{(1)}-{}^{(a)}N_{\boldsymbol{K}}^{(2)}-{}^{(b)}N_{-\boldsymbol{K}}^{(2)}+{}^{(b)}N_{-\boldsymbol{K}}^{(1)}, \tag{11}$$

where ${}^{(a)}N_{\boldsymbol{K}}^{(i)}=a_{\boldsymbol{K}}^{(i)*}a_{\boldsymbol{K}}^{(i)}$ and ${}^{(b)}N_{\boldsymbol{K}}^{(i)}=b_{\boldsymbol{K}}^{(i)*}b_{\boldsymbol{K}}^{(i)}$. (7), (9), (10) and (11) enable us to interpret $a_{\boldsymbol{K}}^{(i)*}$ and $b_{-\boldsymbol{K}}^{(i)*}$ as creation operators for the field quanta specified with their respective energies, momenta, and spin directions listed as follows:

	energy	momentum	spin direction
$a_{\boldsymbol{K}}^{(1)*}$:	k_0	$\boldsymbol{K}$	$+z$
$a_{\boldsymbol{K}}^{(2)*}$:	k_0	$\boldsymbol{K}$	$-z$
$b_{-\boldsymbol{K}}^{(1)*}$:	k_0	$-\boldsymbol{K}$	$+z$
$b_{-\boldsymbol{K}}^{(2)*}$:	k_0	$-\boldsymbol{K}$	$-z$.

* The system of units in which $\hbar=c=1$ is used.

From this and (8) it is clear that $b_{\boldsymbol{K}}^{i)*}$ corresponds to the creation operators for the antiparticle (hole). In the following, e. g. in (14), we understand a^*'s and b^*'s as creation operators for electrons and antineutrinos (or neutrinos and positrons), respectively.

It should be noted that these explicit interpretations are valid only for the special case in which $\boldsymbol{K}$ is parallel to z axis, since otherwise Hamilton function $\alpha\boldsymbol{K}+\beta m$ does not commute with spin operator and hence the energy and z–component of spin cannot take the simultaneous eigenvalues. In the following discussions, however, we always consider the processes in the center of mass system so that we can make these explicit interpretations.

These complications do not occur for the π–meson fields. Following the familiar procedure, one obtains creation operator $c_{\boldsymbol{K}}^{(l)*}$ specified with the momentum and electric charge of the quantum.

Now we introduce the vacuum state vector defined by*

$$\begin{aligned} &{}^{(a)}N_{\boldsymbol{K}}^{(i)}|0>={}^{(b)}N_{\boldsymbol{K}}^{(i)}|0>=0\,, \qquad \text{for any } \boldsymbol{K} \text{ and } i=1,\,2\,, \\ &{}^{(c)}N_{\boldsymbol{K}}^{(l)}|0>=0\,, \qquad \text{for any } \boldsymbol{K} \text{ and } l=1,\,0,\,-1\,, \end{aligned} \tag{12}$$

where ${}^{(c)}N_{\boldsymbol{K}}^{(l)}=c_{\boldsymbol{K}}^{(l)*}c_{\boldsymbol{K}}^{(l)}$ is the occupation number operator for the quantum of the meson field with momentum $\boldsymbol{K}$ and electric charge l in unit of e.

With these notations, one can now express various states in terms of creation operators and vacuum states. Thus

$$|\pi_0^{(l)}>=c_0^{(l)*}|0> \tag{13}$$

is the state in which a π–meson with electric charge l is present at rest. Further,

$$\begin{aligned} &|\uparrow_{\boldsymbol{K}}^{a}\uparrow_{-\boldsymbol{K}}^{\bar{b}}>=a_{\boldsymbol{K}}^{(1)*}b_{-\boldsymbol{K}}^{(1)*}|0>\,, \quad |\uparrow_{\boldsymbol{K}}^{a}\downarrow_{-\boldsymbol{K}}^{\bar{b}}>=a_{\boldsymbol{K}}^{(1)*}b_{-\boldsymbol{K}}^{(2)*}|0>\,, \\ &|\downarrow_{\boldsymbol{K}}^{a}\uparrow_{-\boldsymbol{K}}^{\bar{b}}>=a_{\boldsymbol{K}}^{(2)*}b_{-\boldsymbol{K}}^{(1)*}|0>\,, \quad |\downarrow_{\boldsymbol{K}}^{a}\downarrow_{-\boldsymbol{K}}^{\bar{b}}>=a_{\boldsymbol{K}}^{(2)*}b_{-\boldsymbol{K}}^{(2)*}|0> \end{aligned} \tag{14}$$

are the states in which one a and one $\bar{b}$ (anti)–particle are present with their momenta and spin directions specified in the center of mass system. Thus $|\uparrow_{\boldsymbol{K}}^{a}\uparrow_{-\boldsymbol{K}}^{\bar{b}}>$ is the state in which a and $\bar{b}$ are moving with their respective momenta $\boldsymbol{K}$, and $-\boldsymbol{K}$, and spins both parallel to $+z$ direction, and so on. Note that the arrows in ket symbols describe the spin direction relative to $+z$ direction and not to respective momenta.

The initial state in which a V–particle is present at rest are expressed as

$$|\uparrow_0^{v}>=v_0^{(1)*}|0>\,, \text{ and } |\downarrow_0^{v}>=v_0^{(2)*}|0>\,. \tag{15}$$

Finally for the states in which a π–meson and a Fermion d are present, one has

$$|\uparrow_{\boldsymbol{K}}^{d}\pi_{-\boldsymbol{K}}^{(l)}>=d_{\boldsymbol{K}}^{(1)*}c_{-\boldsymbol{K}}^{(l)*}|0>\,, \text{ and } |\downarrow_{\boldsymbol{K}}^{d}\pi_{-\boldsymbol{K}}^{(l)}>=d_{-\boldsymbol{K}}^{(2)*}c_{-\boldsymbol{K}}^{(l)*}|0>\,. \tag{16}$$

§ 4. Transformation properties and selection rules

We consider three transformations, i. e., rotation through angle φ around z axis, rotation through angle π around x axis, and space inversion. Under these transformations the operators ϕ, ψ and any state vectors undergo unitary transformations.

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* When we have to consider other spin 1/2 fields than a and b–fields, the definition of vacuum states will be extended to include all the fields at hand.

Invariance under space rotation

$$x_i' = \sum_{j=1}^{3} \rho_{ij} x_j , \tag{17}$$

requires

$$R_\rho \phi(x, y, z) R_\rho^{-1} = \phi(x', y', z') , \tag{18}$$

and

$$R_\rho \psi(x, y, z) R_\rho^{-1} = S(\rho) \psi(x', y', z') , \tag{19}$$

where R_ρ is the unitary transformation corresponding to the rotation (17), and $S(\rho)$ represents the spinor transformation.

For inversion

$$x_i' = -x_i , \quad i = 1, 2, 3 , \tag{20}$$

one has

$$P\phi(x, y, z) P^{-1} = \pm \phi(x', y', z') , \tag{21}$$

where upper and lower signs correspond to scalar and pseudoscalar π-meson fields, respectively. On the other hand, ψ transforms as

$$P\psi(x, y, z) P^{-1} = \pm \beta \psi(x', y', z') , \tag{22}$$

or

$$P\psi(x, y, z) P^{-1} = \pm i \beta \psi(x', y', z') . \tag{23}$$

(22) and (23) correspond to ψ–field with real and imaginary parities, respectively. It should be noted that the effect of double signs appear only when two or more ψ–fields are present (see reference 5).

(a) *Decay of π–mesons*

Using (13), (18) and (21), one obtains

$$\begin{aligned} &R_\varphi | \pi_0^{(l)} > = R_\varphi c_0^{(l)*} R_\varphi^{-1} R_\varphi | 0 > = | \pi_0^{(l)} > , \\ &R_\xi | \pi_0^{(l)} > = | \pi_0^{(l)} > , \quad P | \pi_0^{(l)} > = \pm | \pi_0^{(l)} > , \end{aligned} \tag{24}$$

where R_φ and R_ξ denote rotations through angle φ around z axis and through angle π around x axis, respectively. Thus the initial state $| \pi_0^{(l)} >$ is the eigenstate of space rotation and inversion belonging to eigenvalues $+1$ and ± 1, respectively. We have now only to find out if there are any final states with these properties.

First we investigate transformation properties of final states (14) under rotation R_φ defined by

$$\begin{aligned} x' &= x \cos\varphi + y \sin\varphi , \\ y' &= -x \sin\varphi + y \cos\varphi , \end{aligned} \tag{25}$$

for which spinor transformation $S(\varphi)$ of (19) is

$$S(\varphi) = \cos\frac{\varphi}{2} - \alpha_x \alpha_y \sin\frac{\varphi}{2} . \tag{26}$$

This, together with (5) and (19), gives

$$\begin{aligned} &R_\varphi a_{\boldsymbol{K}}^{(1)} R_\varphi^{-1} = e^{-i(\varphi/2)} a_{\boldsymbol{K}}^{(1)} , \quad R_\varphi a_{\boldsymbol{K}}^{(2)} R_\varphi^{-1} = e^{i(\varphi/2)} a_{\boldsymbol{K}}^{(2)} , \\ &R_\varphi b_{-\boldsymbol{K}}^{(1)*} R_\varphi^{-1} = e^{i(\varphi/2)} b_{-\boldsymbol{K}}^{(1)*} , \quad R_\varphi b_{-\boldsymbol{K}}^{(2)*} R_\varphi^{-1} = e^{-i(\varphi/2)} b_{-\boldsymbol{K}}^{(2)*} , \end{aligned} \tag{27}$$

for $\boldsymbol{K}$ parallel to z axis, from which one deduces that

$$R_\varphi a_{\boldsymbol{K}}^{(1)*} b_{-\boldsymbol{K}}^{(1)*} R_\varphi^{-1} = a_{\boldsymbol{K}}^{(1)*} b_{-\boldsymbol{K}}^{(1)*} e^{i\varphi}, \quad R_\varphi a_{\boldsymbol{K}}^{(1)*} b_{-\boldsymbol{K}}^{(2)*} R_\varphi^{-1} = a_{\boldsymbol{K}}^{(1)*} b_{-\boldsymbol{K}}^{(2)*},$$
$$R_\varphi a_{\boldsymbol{K}}^{(2)*} b_{-\boldsymbol{K}}^{(1)*} R_\varphi^{-1} = a_{\boldsymbol{K}}^{(2)*} b_{-\boldsymbol{K}}^{(1)*}, \quad R_\varphi a_{\boldsymbol{K}}^{(2)*} b_{-\boldsymbol{K}}^{(2)*} R_\varphi^{-1} = a_{\boldsymbol{K}}^{(2)*} b_{-\boldsymbol{K}}^{(2)*} e^{-i\varphi}. \tag{28}$$

Thus, for the states represented as (14), one obtains the results:

$$R_\varphi |\uparrow_{\boldsymbol{K}}^a \uparrow_{-\boldsymbol{K}}^{\bar b}> = e^{i\varphi} |\uparrow_{\boldsymbol{K}}^a \uparrow_{-\boldsymbol{K}}^{\bar b}>, \quad R_\varphi |\uparrow_{\boldsymbol{K}}^a \downarrow_{-\boldsymbol{K}}^{\bar b}> = |\uparrow_{\boldsymbol{K}}^a \downarrow_{-\boldsymbol{K}}^{\bar b}>,$$
$$R_\varphi |\downarrow_{\boldsymbol{K}}^a \uparrow_{-\boldsymbol{K}}^{\bar b}> = |\downarrow_{\boldsymbol{K}}^a \uparrow_{-\boldsymbol{K}}^{\bar b}>, \quad R_\varphi |\downarrow_{\boldsymbol{K}}^a \downarrow_{-\boldsymbol{K}}^{\bar b}> = e^{-i\varphi} |\downarrow_{\boldsymbol{K}}^a \downarrow_{-\boldsymbol{K}}^{\bar b}>. \tag{29}$$

Comparing this with (24), it is clear that we now have only to do with the states $|\uparrow_{\boldsymbol{K}}^a \downarrow_{-\boldsymbol{K}}^{\bar b}>$ and $|\downarrow_{\boldsymbol{K}}^a \uparrow_{-\boldsymbol{K}}^{\bar b}>$.

Now we proceed on similar ways to the case of rotation through angle π around x axis,

$$x' = x, \quad y' = -y, \quad z' = -z, \tag{30}$$

for which spinor transformation is found to be

$$S(\xi) = -\sigma_y \sigma_z. \tag{31}$$

It is easily seen that

$$R_\xi a_{\boldsymbol{K}}^{(1)} R_\xi^{-1} = -i a_{-\boldsymbol{K}}^{(2)}, \quad R_\xi a_{\boldsymbol{K}}^{(2)} R_\xi^{-1} = -i a_{-\boldsymbol{K}}^{(1)},$$
$$R_\xi b_{-\boldsymbol{K}}^{(1)*} R_\xi^{-1} = -i b_{\boldsymbol{K}}^{(2)*}, \quad R_\xi b_{-\boldsymbol{K}}^{(2)*} R_\xi^{-1} = -i b_{\boldsymbol{K}}^{(1)*}, \tag{32}$$

and hence

$$R_\xi |\downarrow_{\boldsymbol{K}}^a \uparrow_{-\boldsymbol{K}}^{\bar b}> = |\uparrow_{-\boldsymbol{K}}^a \downarrow_{\boldsymbol{K}}^{\bar b}>, \quad R_\xi |\uparrow_{\boldsymbol{K}}^a \downarrow_{-\boldsymbol{K}}^{\bar b}> = |\downarrow_{-\boldsymbol{K}}^a \uparrow_{\boldsymbol{K}}^{\bar b}>. \tag{33}$$

Finally the inversion (20) will be investigated. For this purpose one is obliged to consider four cases as discussed in Section 2 (a). Transformation properties of a's and b^*'s are

$$P a_{\boldsymbol{K}}^{(i)} P^{-1} = \pm a_{-\boldsymbol{K}}^{(i)}, \quad P b_{-\boldsymbol{K}}^{(i)*} P^{-1} = \mp b_{\boldsymbol{K}}^{(i)*}, \quad \text{for case (A)},$$
$$P a_{\boldsymbol{K}}^{(i)} P^{-1} = \pm a_{-\boldsymbol{K}}^{(i)}, \quad P b_{-\boldsymbol{K}}^{(i)*} P^{-1} = \pm i b_{\boldsymbol{K}}^{(i)*}, \quad \text{for case (B)},$$
$$P a_{\boldsymbol{K}}^{(i)} P^{-1} = \pm i a_{-\boldsymbol{K}}^{(i)}, \quad P b_{-\boldsymbol{K}}^{(i)*} P^{-1} = \pm i b_{\boldsymbol{K}}^{(i)*}, \quad \text{for case (C)},$$
$$P a_{\boldsymbol{K}}^{(i)} P^{-1} = \pm i a_{-\boldsymbol{K}}^{(i)}, \quad P b_{-\boldsymbol{K}}^{(i)*} P^{-1} = \mp i b_{\boldsymbol{K}}^{(i)*}, \quad \text{for case (D)}, \tag{34}$$

and hence

$$P |\uparrow_{\boldsymbol{K}}^a \downarrow_{-\boldsymbol{K}}^{\bar b}> = \mp |\uparrow_{-\boldsymbol{K}}^a \downarrow_{\boldsymbol{K}}^{\bar b}>, \quad P |\downarrow_{\boldsymbol{K}}^a \uparrow_{-\boldsymbol{K}}^{\bar b}> = \mp |\downarrow_{-\boldsymbol{K}}^a \uparrow_{\boldsymbol{K}}^{\bar b}>, \tag{35}$$

where upper signs correspond to the cases (A) and (C)*, while lower ones to cases (B) and (D). It should be remarked that z–component of spin does not change sign under inversion. This rather strange conclusion comes from the fact that a spin vector is an axial one in contrast with a momentum vector $\boldsymbol{K}$.

From (24), (29), (33) and (35) one sees that the final states which must be taken into account are $|\uparrow_{\boldsymbol{K}}^a \downarrow_{-\boldsymbol{K}}^{\bar b}>$, $|\uparrow_{-\boldsymbol{K}}^a \downarrow_{\boldsymbol{K}}^{\bar b}>$, $|\downarrow_{\boldsymbol{K}}^a \uparrow_{-\boldsymbol{K}}^{\bar b}>$ and $|\downarrow_{-\boldsymbol{K}}^a \uparrow_{\boldsymbol{K}}^{\bar b}>$. Of all linear combinations constructed from these four states,

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* Thus the positronium, for example, has always odd *intrinsic parity*. This conclusion is independent of the real-imaginary character of the parity of electron field. See reference 4.

$$|S_1\rangle = |\uparrow^a_{\boldsymbol{K}} \downarrow^{\bar{b}}_{-\boldsymbol{K}}\rangle + |\uparrow^a_{-\boldsymbol{K}} \downarrow^{\bar{b}}_{\boldsymbol{K}}\rangle + |\downarrow^a_{\boldsymbol{K}} \uparrow^{\bar{b}}_{-\boldsymbol{K}}\rangle + |\downarrow^a_{-\boldsymbol{K}} \uparrow^{\bar{b}}_{\boldsymbol{K}}\rangle$$

and

$$|S_2\rangle = |\uparrow^a_{\boldsymbol{K}} \downarrow^{\bar{b}}_{-\boldsymbol{K}}\rangle - |\uparrow^a_{-\boldsymbol{K}} \downarrow^{\bar{b}}_{\boldsymbol{K}}\rangle - |\downarrow^a_{\boldsymbol{K}} \uparrow^{\bar{b}}_{-\boldsymbol{K}}\rangle + |\downarrow^a_{-\boldsymbol{K}} \uparrow^{\bar{b}}_{\boldsymbol{K}}\rangle \qquad (36)$$

are left to have the same transformation properties as $|\pi^{(l)}_0\rangle$. The final selection rules for π–meson decays are listed in Table I, from which one sees that the decay process $\pi \to a + \bar{b}$ is allowed for any parities of π–mesons and for any possible assignments of various parities to a and b fields. Needless to say, a and b must be chosen so that these processes are consistent with charge conservation.

Table I. Selection rules for π–meson decay

parity of π	parity of (a, b)	allowed final state
1	cases (A) and (C)	S_2
1	cases (B) and (D)	S_1
−1	cases (A) and (C)	S_1
−1	cases (B) and (D)	S_2

The allowed final states $|S_1\rangle$ and $|S_2\rangle$ seem, at first sight, to be symmetric for the exchange of two final particles a and $\bar{b}$. One might think $|S_1\rangle$ corresponds to ${}^3S$ and $|S_2\rangle$ to ${}^1P$ state. It is shown in Appendix, however, that this is not true. There one will see that $|S_1\rangle$ and $|S_2\rangle$ correspond to ${}^1S$ and ${}^3P$ states respectively as the case must be.

(β) *Decay of V^0–particles*

By virtue of (15), (27) and (32) with $\boldsymbol{K}=0$, one obtains

$$R_\varphi|\uparrow^v_0\rangle = e^{i(\varphi/2)}|\uparrow^v_0\rangle, \quad R_\varphi|\downarrow^v_0\rangle = e^{-i(\varphi/2)}|\downarrow^v_0\rangle,$$
$$R_\xi|\uparrow^v_0\rangle = i|\downarrow^v_0\rangle, \quad R_\xi|\downarrow^v_0\rangle = i|\uparrow^v_0\rangle. \qquad (37)_1$$

Further

$$P|\uparrow^v_0\rangle = |\uparrow^v_0\rangle, \quad P|\downarrow^v_0\rangle = |\downarrow^v_0\rangle \qquad (37)_2$$

for cases (A)′ and (B)′, and

$$P|\uparrow^v_0\rangle = -i|\uparrow^v_0\rangle, \quad P|\downarrow^v_0\rangle = -i|\downarrow^v_0\rangle \qquad (37)_3$$

for cases (C)′ and (D)′.

These are the transformation properties of initial states and we are now to find out what will result for final states. The treatments are quite similar to those made in (α) of this section and one readily sees for R_φ and R_ξ

$$R_\varphi|\uparrow^a_{\boldsymbol{K}}\pi^{(l)}_{-\boldsymbol{K}}\rangle = e^{i(\varphi/2)}|\uparrow^a_{\boldsymbol{K}}\pi^{(l)}_{-\boldsymbol{K}}\rangle, \quad R_\varphi|\downarrow^a_{\boldsymbol{K}}\pi^{(l)}_{-\boldsymbol{K}}\rangle = e^{-i(\varphi/2)}|\downarrow^a_{\boldsymbol{K}}\pi^{(l)}_{-\boldsymbol{K}}\rangle,$$

and

$$R_\xi|\uparrow^a_{\boldsymbol{K}}\pi^{(l)}_{-\boldsymbol{K}}\rangle = i|\downarrow^a_{-\boldsymbol{K}}\pi^{(l)}_{\boldsymbol{K}}\rangle, \quad R_\xi|\downarrow^a_{\boldsymbol{K}}\pi^{(l)}_{-\boldsymbol{K}}\rangle = i|\uparrow^a_{-\boldsymbol{K}}\pi^{(l)}_{\boldsymbol{K}}\rangle. \qquad (38)$$

On the other hand, for space inversion, one has eight possible cases as discussed at the end of Section 2. Thus

$$
\begin{aligned}
P|\uparrow^{d}_{K}\pi^{(l)}_{-K}> &= \pm|\uparrow^{d}_{-K}\pi^{(l)}_{K}>, && \text{for case (A)}',\\
&= \mp|\uparrow^{d}_{-K}\pi^{(l)}_{K}>, && \text{for case (B)}',\\
&= \mp i|\uparrow^{d}_{-K}\pi^{(l)}_{K}>, && \text{for case (C)}',\\
&= \pm i|\uparrow^{d}_{-K}\pi^{(l)}_{K}>, && \text{for case (D)}', \qquad (39)_1
\end{aligned}
$$

and

$$
\begin{aligned}
P|\downarrow^{d}_{K}\pi^{(l)}_{-K}> &= \pm|\downarrow^{d}_{-K}\pi^{(l)}_{K}>, && \text{for case (A)}',\\
&= \mp|\downarrow^{d}_{-K}\pi^{(l)}_{K}>, && \text{for case (B)}',\\
&= \mp i|\downarrow^{d}_{-K}\pi^{(l)}_{K}>, && \text{for case (C)}',\\
&= \pm i|\downarrow^{d}_{-K}\pi^{(l)}_{K}>, && \text{for case (D)}', \qquad (39)_2
\end{aligned}
$$

where upper and lower signs correspond to scalar and pseudoscalar mesons, respectively.

(37), (38) and (39) show that the final states one should take into account are the following four:

$$
\begin{aligned}
|T_1> &= |\uparrow^{d}_{K}\pi^{(l)}_{-K}> + |\uparrow_{-K}\pi^{(l)}_{K}>, \quad |T_2> = |\uparrow^{d}_{K}\pi^{(l)}_{-K}> - |\uparrow^{d}_{-K}\pi^{(l)}_{K}>,\\
|T_3> &= |\downarrow^{d}_{K}\pi^{(l)}_{-K}> + |\downarrow^{d}_{-K}\pi^{(l)}_{K}>, \quad |T_4> = |\downarrow^{d}_{K}\pi^{(l)}_{-K}> - |\downarrow^{d}_{-K}\pi^{(l)}_{K}>. \qquad (40)
\end{aligned}
$$

Before deducing the final selection rules, one has to recall the fact that the parity of a π–meson is closely related to that of a nucleon as remarked in Section 2 (a). With this consideration, the selection rules for the decay of V^0–particle are summarized in Table II. It is clear from the table that, though we have many possible assignments of various parities, yet none of the V^0–decay schemes can be made forbidden.

Table II. Selection rules for V^0–decay

parity				allowed final state	
P	N	π	V^0	$V^0\to N+\pi^0$	$V^0\to P+\pi^-$
1	1	−1	1	T_2, T_4	T_2, T_4
1	−1	1	1	T_2, T_4	T_1, T_3
−1	1	1	1	T_1, T_3	T_2, T_4
−1	−1	−1	1	T_1, T_3	T_1, T_3
i	i	1	i	T_1, T_3	T_1, T_3
i	$-i$	−1	i	T_1, T_3	T_2, T_4
$-i$	i	−1	i	T_2, T_4	T_1, T_3
$-i$	$-i$	1	i	T_2, T_4	T_2, T_4

We have also investigated the process in which a Fermion decays to give rise to a Fermion and a γ in the final state. Characterizing an outgoing photon with its direction of circular polarization and proceeding on quite similar ways, it was concluded that, for any reasonable assignments of parities to the initial and final Fermions, there exists no process which is forbidden. This conclusion is, however, not so serious as in case of π or V^0–decay considered above, since the process of γ–emission is easily forbidden (or at least improbable) if we assume no direct couplings between these Fermions and electromagnetic fields.

§ 5. Charge independence hypothesis

The purpose of our investigation made in the preceding section was to find out: whether there exist any possibilities to forbid the decay of a π–meson into an electron-neutrino pair when we adopt the original Yukawa theory in which the interactions between nucleons and leptons are considered to be transmitted by π–meson field. If the interactions between nucleons and π–meson field can be assumed to be charge independent,[8] it would be also natural to introduce the hypothesis of charge independent interaction between leptons and π–meson field. For this purpose one has only to introduce a charge symmetric coupling between lepton and π–meson fields. The net effect of this hypothesis is that isotopic angular momentum is now a good quantum number and hence must be conserved throughout the decay process.

Let us make the following assignments of isotopic spin τ and its z–component τ_z for leptons, π–mesons, and nucleons:

	electron	neutrino	π^-	π^0	π^+	N	P
τ :	1/2	1/2	1	1	1	1/2	1/2
τ_z :	1/2	−1/2	1	0	−1	1/2	−1/2.

(41)

It is clear here that the system which consists of an electron and a neutrino has $\tau_z=0$ and hence the disintegration of a charged π–meson into these constituents cannot occur. However, since an antiparticle may be considered to have the oppositely directed isotopic spin[9], antineutrinos, for example, are in the same isotopic spin state as electrons. Thus a π^-–meson can only disintegrate into an electron and antineutrino. It should be noted here that an unobserved particle accompanying an electron in ordinary β–decay process must be an antineutrino and not neutrino in so far as one adopts original Yukawa theory with charge independence hypothesis, although this point has been considered as only the problem of definition thus far. A π^+–meson, on the other hand, can decay into an antielectron (positron) and a neutrino (not antineutrino).

Now the wave function for the two-lepton systems which results from the decay of a charged π–meson may be written in the form:

$$\begin{pmatrix}\textit{isotopic spin}\\ \textit{function}\end{pmatrix}\cdot\begin{pmatrix}\textit{spin}\\ \textit{function}\end{pmatrix}\cdot\begin{pmatrix}\textit{coordinate}\\ \textit{function}\end{pmatrix}. \qquad (42)$$

The first factor is symmetric for the exchange of two leptons, since one of them is the anti-lepton and hence has the same τ_z as the other.[9] Last two factors are given by Eq. (36) and are antisymmetric as deduced in Appendix. Thus the product of three factors (42) is antisymmetric for the exchange of final two leptons. If one assumes a π–meson to be vector it follows that the allowed final state is ${}^3S$ (see Appendix). In this case (42) is symmetric and one might imagine that the two-lepton decay of a vector meson is forbidden on account of the exclusion principle. However, this is not the case when one of the two leptons is anti, as remarked by the present authors.[9]

Thus the introduction of the charge independence hypothesis cannot make the situation better at all and we must conclude that the two-lepton decay of a charged π–meson

cannot be forbidden any way in so far as one takes the original Yukawa type interaction. This conclusion casts considerable doubts on our model to consider μ–mesons as the excited states of leptons as was mentioned in Section 1. It should be added, however, that nothing is yet said about the quantitative nature of the excitation of leptons up to μ–mesons and hence our model is not completely denied. Some factors, of which we know nothing yet, might work to reduce the probability of the π–meson decay into two leptons negligibly small compared with that of $\pi \rightarrow (\mu, \nu)$ decay scheme.

Here we shall investigate what will follow of the decay of a π–meson from various assignments of isotopic angular momenta to μ–mesons. If one considers μ–mesons as the charge excited states of leptons the most natural possibility is to assign $\tau = 3/2$ for μ–mesons. One can then assign μ^{--}, μ^{-}, μ^{0}, μ^{+} to the states with $\tau = 3/2$, $1/2$, $-1/2$ and $-3/2$, respectively. For these assignments with (41), the process

$$\pi^{\pm} \rightarrow \mu^{\pm} + \bar{\nu} \quad (anti)$$

is allowed. One must note, however, that the processes

$$\pi^{+} \rightarrow \mu^{0} + \bar{e} \quad (anti), \text{ and } \pi^{-} \rightarrow \mu^{--} + \bar{e} \quad (anti),$$

can also occur and these assignments of isotopic spins to μ–mesons lead to difficulty. One can also assume that isotopic spin of a μ–meson is $1/2$. In this case there are three possible assignments of μ–mesons to two eigenvalues of τ_z, i. e., $1/2$ and $-1/2$. They are :

τ_z	*case* (*i*)	*case* (*ii*)	*case* (*iii*)
$1/2$	μ^{0}	μ^{-}	μ^{-}
$-1/2$	μ^{+}	μ^{0}	μ^{+} .

Let us investigate these three possible cases separately.

Case (*i*) : For this assignment one is to consider μ^{-}'s as anti-particles of μ^{+}–mesons. The decay schemes

$$\pi^{-} \rightarrow \bar{\mu}^{+} \quad (anti) + \bar{\nu} \quad (anti)$$

and

$$\pi^{+} \rightarrow \mu^{+} \quad (not\ anti) + \nu \quad (not\ anti)$$

are allowed. This spoils the symmetry of the theory and moreover the processes

$$\pi^{-} \rightarrow \mu^{0} + e \quad \text{and} \quad \pi^{+} \rightarrow \bar{\mu}^{0} + \bar{e}$$

should occur and conflict with our experimental knowledge.

Case (*ii*) : μ^{+} is considered to be the antiparticle of μ^{-}. This assignment allows the processes

$$\pi^{-} \rightarrow \mu^{-} + \bar{\nu} \quad (anti) \quad \text{and} \quad \pi^{+} \rightarrow \bar{\mu}^{-} \quad (anti) + \nu$$

which are similar to ordinary pair creation processes. One must, however, also allow for the decay modes

$$\pi^{-} \rightarrow \bar{\mu}^{0} \quad (anti) + e \quad \text{and} \quad \pi^{+} \rightarrow \mu + \bar{e} \quad (anti)$$

which lead to the similar difficulty to *case* (*i*).

Case (iii) : In this case *one needs not assume the existence of μ^0–mesons.* Isotopic angular momentum is conserved for the processes

$$\pi^- \to \mu^- + \bar{\nu}\ (anti) \quad \text{and} \quad \pi^+ \to \mu^+ + \nu\ (not\ anti).$$

There are no other possible decay modes. This set of processes seems to spoil the symmetry at first sight, yet if one recalls the μ–decays

$$\mu^- \to \nu + e + \bar{\nu}\ (anti)$$

and

$$\mu^+ \to \bar{\nu}\ (anti) + \bar{e}\ (anti) + \nu\,, \tag{43}$$

this apparent asymmetry turns out to be of no matter. This point is clearly understood if one assumes μ^- and μ^+–mesons to be excited states of neutrinos and antineutrinos, respectively. We have been, however, on the stand point of charge symmetry hypothesis and hence it would be rather unnatural to consider μ–mesons as the excited states of neutrinos (or antineutrinos) and not leptons (generic terms including electrons and neutrinos symmetrically). Thus one has also to put the same weight for the processes

$$\mu^- \to e + \bar{e} + e$$

and

$$\mu^+ \to \bar{e} + e + \bar{e} \tag{44}$$

as for (43). This expectation that the process (44) will occur with the probability of the same order as (43) is the great difficulty of our model.

Finally let us investigate the effect of the charge independence hypothesis on the decay of V–particles. If one assumes that V–particles are the excited states of nucleons through their interactions with π–meson field and that this interaction is charge symmetric, the isotopic angular momentum must be conserved throughout any decay processes of V–particles. It is well known that the two-body decays of V–particles are allowed if one assumes $\tau = 3/2$ for V–particles. We shall disregard this assignment of isotopic angular momentum, since no particles which correspond to the states of higher charge are found. If one assumes a V–particle has the isotopic angular momentum $\tau = 1/2$, there are two reasonable assignments of V–particles of different charges. First let us assign V^0 and V^+ to $\tau_z = 1/2$ and $-1/2$, respectively. In this case the decay modes

$$V^0 \to N + \pi^0, \quad \text{or} \quad \to P + \pi^-,$$
$$V^+ \to P + \pi^0, \quad \text{or} \quad \to N + \pi^+,$$

and the three-body decays, for example

$$V^0 \to N + \pi^+ + \pi^-, \quad \text{or} \quad \to P + \pi^- + \pi^0 \tag{45}$$

are allowed at the same time. *Remember we have here assumed that no V^- exists.* If, on the contrary, there exists V^- and V^0 (and no V^+),

$$V^0 \to N + \pi^0, \quad \text{or} \quad \to P + \pi^-,$$
$$V^- \to N + \pi^-$$

are all forbidden, as easily seen from the assignment of V^- and V^0 to $\tau_z = 1/2$ and $-1/2$, respectively. In this case, however, the favorable three-body decays (45) are also forbidden by the requirement of the isotopic angular momentum conservation. Since the

decay of a V^0 is experimentally established (though its decay scheme is not quite clear), one can definitely say, in so far as he takes charge independence hypothesis, that: V^+ must exist any way. If non-existence of V^- is established, V–particles must have $\tau=1/2$. If, on the contrary, the existence of V^- is established, V–particles must have $\tau=3/2$ or larger. This point has also been noted by Watson.[8]

Thus one is led to the conclusion that it would be difficult to forbid the two-body decays of V–particles by means of selection rules without introducing any higher spin or isotopic spin values. As the final remark on the decays of V–particles we would say: if two-body decay of a V–particle does really not occur, it will be more hopeful for its explanation to investigate the probability of different decay schemes solving the problem of excited states rather than to try to make the two-body decays forbidden by means of selection rules assuming higher spin or isotopic spin values.

§ 6. Summary of results

(α) *Decay of π–mesons*

Returning to original Yukawa theory in which the interaction between nucleon and lepton fields is transmitted by π–meson field, we have first investigated if the unobserved decay of π–mesons into two leptons can be forbidden by means of general principle of invariance under space rotation and inversion. The conclusion was negative, namely, this decay mode of a π-meson is always allowed with any reasonable assignments of parities to various Fermions in play.

The selection rules thus obtained (Table I) were reexamined from the stand point of charge independence hypothesis. It was concluded that the introduction of this hypothesis cannot better the situation at all.

Decay of a π–meson into a μ–meson and a lepton was investigated under various assignments of isotopic spin angular momenta to μ–mesons. The most favorable one is to assign $\tau_z=1/2$ and $-1/2$ to μ^- and μ^+–mesons, respectively. The charge independence hypothesis requires, however, that unobserved three-electron decay (one or two of them should be anti) must occur with the frequency of the same order as usual decay mode (43), casting considerable doubts on our model to consider μ–mesons as the excited states of leptons which include electrons and neutrinos symmetrically.

New methods capable of treating the problem of excitation of elementary particles are strongly hoped for, which may offer us means to investigate these difficulties more quantitatively.

(β) *Decay of V–particles*

Invariance under space rotation and inversion forbids no two-body (one Fermion and one Boson) decay processes of a V–particle. Discussions under charge independence hypothesis have shown: two and three-body decays of a V–particle are both allowed if one assumes existence of only V^+ and V^0, while both are forbidden if the existence of only V^- and V^0 is assumed. This led to the interesting conclusion on the isotopic angular momenta of V–particles. That is: V^+ must exist. If V^- exists V–particles have $\tau=3/2$ or larger, if does not then $\tau=1/2$.

The means with which one can estimate the frequency of various V–decay processes solving the problem of excited states, are here also strongly hoped for.

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Appendix

Configuration space representation of $|S_1>$ *and* $|S_2>$

Let us try to find the configuration space representatives of states obtained by applying various creation operators $a_{\boldsymbol{K}}^{(\dagger)*}$, $b_{\boldsymbol{K}}^{(\dagger)*}$, etc., to the vacuum state $|0>$ defined by Eq. (12). For this purpose, Fock's treatments[10] are unsatisfactory since this author considers only *one electron theoretical* case, and one should refer to the work of Sato[11] (to be referred to in what follows as I) in which *positron theoretical* generalization is made.

Let the q-number spinor $\psi(\boldsymbol{r})$ be decomposed into two parts as

$$\psi_\alpha(\boldsymbol{r})=\psi_\alpha^{(+)}(\boldsymbol{r})+\psi_\alpha^{(-)}(\boldsymbol{r}), \tag{A·1}$$

where

$$\psi^{(+)}(\boldsymbol{r})=\sum(K^2+k^2)^{-(1/2)}\left\{a_{\boldsymbol{K}}^{(1)}\begin{bmatrix}K\\0\\k_2\\k_1\end{bmatrix}+a_{\boldsymbol{K}}^{(2)}\begin{bmatrix}0\\K\\k_2\\-k_3\end{bmatrix}\right\}e^{i\boldsymbol{K}\boldsymbol{r}},$$

$$\psi^{(-)}(\boldsymbol{r})=\sum(K^2+k^2)^{-(1/2)}\left\{b_{-\boldsymbol{K}}^{(2)*}\begin{bmatrix}-k_3\\-k_1\\K\\0\end{bmatrix}+b_{\boldsymbol{K}}^{(1)*}\begin{bmatrix}-k_2\\k_3\\0\\K\end{bmatrix}\right\}e^{i\boldsymbol{K}\boldsymbol{r}}, \tag{A·2}$$

following Eqs. (5) and (6). $\psi^{(-)}(\boldsymbol{r})$ is to be interpreted to create an antiparticle. Now the probability amplitude (wave function) of finding n particles (space coordinates $\boldsymbol{x}_i$, spin coordinates α_i) and m antiparticles (space coordinates $\boldsymbol{y}_j$, spin coordinates β_j) in a state represented by $|\Psi>$ is

$$\langle \boldsymbol{x}_1\alpha_1, \boldsymbol{x}_2\alpha_2,\cdots, \boldsymbol{x}_n\alpha_n\,;\,\boldsymbol{y}_1\beta_1,\cdots,\boldsymbol{y}_m\beta_m|\Psi\rangle.$$

Hence the configuration space wave function of the state in which one antiparticle is found is written as

$$\langle 0\,;\,\boldsymbol{y}_1\beta_1|\psi_\alpha^{(-)}(\boldsymbol{r})|0\rangle\equiv\langle 0\,;\,\boldsymbol{y}_1\beta_1|\psi_\alpha^{(-)}(\boldsymbol{r})|0\,;\,0\rangle.$$

According to Eq. (9) of I, we have

$$\langle 0\,;\,\boldsymbol{y}_1\beta_1|\psi_\alpha^{(-)}(\boldsymbol{r})|0\,;\,0\rangle=S_{\alpha\beta_1}^{(-)}(\boldsymbol{r}-\boldsymbol{y}_1), \tag{A·3}$$

where $S^{(-)}(\boldsymbol{x})$ is the function obtained by putting $x_0=0$ in Schwinger's[12] $S^{(-)}(x_\mu)$. Introducing a creation operator of a particle

$$\bar{\psi}^{(-}\equiv\psi^{(+)*}\beta, \tag{A·4}$$

the wave function of the state in which one ordinary and one antiparticle are present is given by

$$\langle \boldsymbol{x}_1\alpha_1\,;\,\boldsymbol{y}_1\beta_1\,|\,\bar{\psi}^{(-)}_{\alpha'}(\boldsymbol{r}')\psi^{(-)}_{\alpha}(\boldsymbol{r})\,|\,0\rangle$$
$$=\sum_{\beta_1'}\int\langle \boldsymbol{x}_1\alpha_1\,;\,\boldsymbol{y}_1\beta_1\,|\,\bar{\psi}^{(-)}_{\alpha'}(\boldsymbol{r}')\,|\,0\,;\,\boldsymbol{y}_1'\beta_1'\rangle d\boldsymbol{y}_1'\langle 0\,;\,\boldsymbol{y}_1'\beta_1'\,|\,\psi^{(-)}_{\alpha}(\boldsymbol{r})\,|\,0\,;\,0\rangle. \qquad (A\cdot5)$$

Taking account of Eq. (A·3) and Eq. (10) of I, namely

$$\langle \boldsymbol{x}_1\alpha_1\,;\,\boldsymbol{y}_1\beta_1\,|\,\bar{\psi}^{(-)}_{\alpha'}(\boldsymbol{r}')\,|\,0\,;\,\boldsymbol{y}_1'\beta_1'\rangle$$
$$=-(\beta S^{(+)}(\boldsymbol{x}_1-\boldsymbol{r}'))_{\alpha_1\alpha'}\delta(\boldsymbol{y}_1-\boldsymbol{y}_1')\delta_{\beta_1\beta_1'}, \qquad (A\cdot6)$$

where[12]

$$S^{(+)}(\boldsymbol{x})=S^{(+)}(x_\mu)\,|_{x_0=0}\,.$$

(A·5) reduces to

$$\langle \boldsymbol{x}_1\alpha_1\,;\,\boldsymbol{y}_1\beta_1\,|\,\bar{\psi}^{(-)}_{\alpha'}(\boldsymbol{r}')\psi^{(-)}_{\alpha}(\boldsymbol{r})\,|\,0\rangle$$
$$=-(\beta S^{(+)}(\boldsymbol{x}_1-\boldsymbol{r}'))_{\alpha_1\alpha'}S^{(-)}_{\alpha\beta_1}(\boldsymbol{r}-\boldsymbol{y}_1). \qquad (A\cdot7)$$

It is more convenient to introduce a slightly different representation (which satisfies ordinary Dirac equation). Following Eq. (27) of I

$$\langle \boldsymbol{x}_1\alpha_1\,;\,\boldsymbol{y}_1\beta_1\,|\,\psi^{(+)*}_{\alpha'}(\boldsymbol{r}')\psi^{(-)}_{\alpha}(\boldsymbol{r})\,|\,0\rangle$$
$$=-(S^{(+)}(\boldsymbol{x}_1-\boldsymbol{r}')\beta)_{\alpha_1\alpha'}(S^{(-)}(\boldsymbol{r}-\boldsymbol{y}_1)C)_{\alpha\beta_1}, \qquad (A\cdot8)$$

where C is a 4–4 matrix satisfying

$$C^{-1}\gamma_\mu C=-\gamma_\mu^T,\quad C^T=-C,\quad C^*C=1\,. \qquad (A\cdot9)$$

Now one is ready to find the configuration space wave function of the states $|S_1>$ and $|S_2>$ given in Eq. (36). One can write

$$\langle \boldsymbol{x}_1\,;\,\boldsymbol{y}_1\,|\,a^{(1)*}_{\boldsymbol{K}}\,b^{(2)*}_{-\boldsymbol{K}}\,|\,0\rangle\equiv\langle \boldsymbol{x}_1\,;\,\boldsymbol{y}_1\,|\uparrow^{a}_{\boldsymbol{K}}\downarrow^{\bar{b}}_{-\boldsymbol{K}}\rangle$$
$$=\langle \boldsymbol{x}_1\,;\,\boldsymbol{y}_1\,|\int d\boldsymbol{r}\int d\boldsymbol{r}'[\psi^{(+)}(\boldsymbol{r}')u^{(1)}_{\boldsymbol{K}}e^{i\boldsymbol{K}\boldsymbol{r}'}][v^{(-)*}_{\boldsymbol{K}}e^{-i\boldsymbol{K}\boldsymbol{r}}\psi^{(-)}(\boldsymbol{r})]\,|\,0\rangle$$
$$=-\left[\int S^{(+)}(\boldsymbol{x}_1-\boldsymbol{r}')\beta u^{(1)}_{\boldsymbol{K}}e^{i\boldsymbol{K}\boldsymbol{r}'}d\boldsymbol{r}'\right]\left[\int v^{(1)*}_{\boldsymbol{K}}S^{(-)}(\boldsymbol{r}-\boldsymbol{y}_1)Ce^{-i\boldsymbol{K}\boldsymbol{r}}d\boldsymbol{r}\right], \qquad (A\cdot10)$$

where we have put

$$u^{(1)}_{\boldsymbol{K}}=\frac{1}{\sqrt{K^2+k^2}}\begin{bmatrix}K\\0\\k_3\\k_1\end{bmatrix},\quad u^{(2)}_{\boldsymbol{K}}=\frac{1}{\sqrt{K^2+k^2}}\begin{bmatrix}0\\K\\k_2\\-k_3\end{bmatrix},$$
$$v^{(1)}_{\boldsymbol{K}}=\frac{1}{\sqrt{K^2+k^2}}\begin{bmatrix}-k_3\\-k_1\\K\\0\end{bmatrix},\quad v^{(2)}_{\boldsymbol{K}}=\frac{1}{\sqrt{K^2+k^2}}\begin{bmatrix}-k_2\\k_3\\0\\K\end{bmatrix}, \qquad (A\cdot11)$$

and use is made of the matrix notation without writing spinor index α and β explicitly. To carry out the integration in (A·10) we note that

$$S^{(-)}(x)=\left(\gamma_\mu\frac{\partial}{\partial x_\mu}-m\right)\Delta^{(-)}(x_\mu)\Big|_{x_0=0}$$
$$=\left(-i\frac{\partial}{\partial x_0}-\alpha\frac{1}{i}\frac{\partial}{\partial x}-\beta m\right)\beta\Delta^{(-)}(x_\mu)\Big|_{x_0=0}$$
$$=\frac{i}{2}\delta(x)\beta-\left(\alpha\frac{1}{i}\frac{\partial}{\partial x}+\beta m\right)\beta\frac{1}{2}\left(\frac{-i}{(2\pi)^3}\right)\int\frac{-1}{\sqrt{k^2+m^2}}e^{iKx}dK,$$

and similarly

$$S^{(+)}(x)=\frac{i}{2}\delta(x)\beta-\left(\alpha\frac{1}{i}\frac{\partial}{\partial x}+\beta m\right)\beta\frac{1}{2}\left(\frac{-i}{(2\pi)^3}\right)\int\frac{+1}{\sqrt{k^2+m^2}}e^{iKx}dK.$$

Further

$$\left(\alpha\cdot\frac{1}{i}\frac{\partial}{\partial x}+\beta m\right)u_K^{(i)}e^{iKx}=\sqrt{k^2+m^2}\,u_K^{(i)}e^{iKx},$$

and

$$v_K^{(i)*}e^{-iKx}\left(-\alpha\frac{1}{i}\frac{\partial}{\partial x}+\beta m\right)=-\sqrt{k^2+m^2}\,v_K^{(i)*}e^{-iKx}.$$

Thus

$$\int v_K^{(1)*}S^{(-)}(r-y_1)Ce^{-iKr}dr$$
$$=\frac{i}{2}v_K^{(1)*}e^{-iKy_1}\beta C-\frac{1}{2}\left(\frac{-i}{(2\pi)^3}\right)\iint dr\,dK\,v_K^{(1)*}e^{-iKr}$$
$$\times\left(-\alpha\frac{1}{i}\frac{\overleftarrow{\partial}}{\partial x}+\beta m\right)\beta C\frac{-1}{\sqrt{k^2+m^2}}e^{iKr}$$
$$=iv_K^{(1)*}e^{-iKy_1}\beta C,$$

and similarly

$$\int S^{(+)}(x_1-r')\beta u_K^{(1)}e^{iKr'}dr'=iu_K^{(1)}e^{iKx_1}.$$

Therefore (A·10) gives

$$\langle x_1;y_1|\uparrow_K^a\downarrow_{-K}^{\bar b}\rangle=(u_K^{(1)}e^{iKx_1})(v_K^{(1)*}e^{-iKy_1}\beta C),\qquad(\text{A}\cdot12)_1$$

and in the same way, for example,

$$\langle x_1;y_1|\downarrow_K^a\uparrow_{-K}^{\bar b}\rangle=(u_K^{(2)}e^{iKx_1})(v_K^{(2)*}e^{-iKy_1}\beta C).\qquad(\text{A}\cdot12)_2$$

It should be remarked here the fact that the obtained Schrödinger wave functions in configuration space (A·12) have no symmetry characters with regard to coordinates of ordinary and anti-particles, despite the anti-commutativity of a_K's and b_K's. This is in contrast with the *one electron theoretical* treatment of Fock's (see, for example, Eq. (8) of *Zweiter Teil*, reference 10). Particles and antiparticles are thus considered to be independent of each other and are *not* subject to exclusion principle. This situation may be understood clearly if one insists that an antiparticle is a hole (not particle). It was pointed out by the present authors[9] that one should introduce so called *antiparticle coordinate* if one is to treat the holes as particles.

Making use of the concrete representation of C, namely

$$C=\gamma_2\gamma_4=iu_2=\begin{vmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{vmatrix},$$

and (A·11), one can readily show the following results:

$$v_K^{(1)\dagger} e^{-iKy_1}\beta C=-C\beta v_K^{(1)*}e^{-iKy_1}=-u_{-K}^{(2)}e^{-iKy_1},$$
$$v_K^{(2)*} e^{-iKy_1}\beta C=-C\beta v_K^{(2)*}e^{-iKy_1}=+u_{-K}^{(1)}e^{-iKy_1}. \qquad (A\cdot 13)$$

Here the difference in signs is essential. One can now write according to (A·10), (A·12) and (A·13),

$$\langle x_1\,;\,y_1\,|\,S_1\rangle=-u_K^{(1)}(a)e^{iKx_1}u_{-K}^{(2)}(\bar{b})e^{-iKy_1}+u_K^{(2)}(a)e^{iKx_1}u_{-K}^{(1)}(\bar{b})e^{-iKy_1}$$
$$-u_{-K}^{(1)}(a)e^{-iKx_1}u_K^{(2)}(b)e^{iKy_1}+u_{-K}^{(2)}(a)e^{-iKx_1}u_K^{(1)}(\bar{b})e^{iKy_1}. \qquad (A\cdot 14)$$

If Pauli approximation is considered to be valid, one may write introducing ordinary spin eigenfunctions α and β as

$$u_K^{(1)}(a)=u_{-K}^{(1)}(a)\equiv\alpha(a),$$
$$u_K^{(2)}(a)=u_{-K}^{(2)}(a)\equiv\beta(a), \quad \text{etc.},$$
$$\langle x_1\,;\,y_1\,|\,S_1\rangle=-(\alpha(a)\beta(\bar{b})-\beta(a)\alpha(\bar{b}))(e^{iK(x_1-y_1)}+e^{-iK(x_1-y_1)}),$$
$$\langle x_1\,;\,y_1\,|\,S_2\rangle=-(\alpha(a)\beta(\bar{b})+\beta(a)\alpha(\bar{b}))(e^{iK(x_1-y_1)}-e^{-iK(x_1-y_1)}). \qquad (A\cdot 15)$$

These may be symbolized as ${}^1S$ and ${}^3P$ states, respectively.

Finally, let us mention the decay of a vector meson (spin directed towards $+z$) into a lepton pair. Assuming the same parity to electrons and neutrinos, the final state is found to be

$$|\,S_3>=|\uparrow_K^a\uparrow_{-K}^b>+|\uparrow_{-K}^a\uparrow_K^b>.$$

The configuration space wave function is

$$\langle x_1\,;\,y_1\,|\,S_3\rangle=u_K^{(1)}(a)e^{iKx_1}u_{-K}^{(1)}(\bar{b})e^{-iKy_1}+u_{-K}^{(1)}(a)e^{-iKx_1}u_K^{(1)}(\bar{b})e^{iKy_1},$$

or, in Pauli approximation,

$$\langle x_1\,;\,y_1\,|\,S_3\rangle=\alpha(a)\alpha(\bar{b})(e^{iK(x_1-y_1)}+e^{-iK(x_1-y_1)}).$$

This may be symbolized as ${}^3S$ state.

References

1) M. Sugawara, Prog. Theor. Phys. **7** (1952), 599.
2) H. L. Friedman and J. Rainwater, Phys. Rev. **84** (1951), 864.
3) R. B. Leighton, S. D. Wanlass and W. L. Alford, Phys. Rev. **83** (1951), 843.
   W. B Fretter, Phys. Rev. **83** (1951), 1053.
4) C. N. Yang, Phys. Rev. **77** (1950), 242.
5) C. N. Yang and J. Tiomno, Phys. Rev. **79** (1950), 495.
6) D. L. Clark, A. Roberts and R. Wilson, Phys. Rev. **85** (1952), 523.
7) Iwanenko and Sokolow, Phys. ZS. Sowj. **11** (1937), 590.
8) K. M. Watson and K. A. Brueckner, Phys. Rev. **83** (1951), 1.
   K. M. Watson, Phys. Rev. **85** (1952), 852.
9) T Hamada and M. Sugawara, Prog. Theor. Phys. **8** (1952), 256.
10) V. Fock, ZS. f. Phys. **75** (1932), 622.
11) I. Sato, Sci. Rep. Tohoku Univ. Series 1, **34** (1950), 75.
12) J. Schwinger, Phys. Rev. **74** (1948), 1439; **75** (1949), 651; **76** (1949), 790.

Letters to the Editor

On the Equivalence of Moment Method and Fourier Transform Method in the Theory of Spectral Line Shape

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The method of moment, due to Van Vleck[1], which offers a very powerful means to analyse the magnetic resonance absorption spectra, can be shown to be equivalent to the method of Fourier transform which is often used in the theory of pressure broadening of spectral lines.[2),3),4)]

Let $g(\omega)$ be the shape function of a spectral line normalized so that

$$\int_0^\infty g(\omega)\,d\omega=0. \qquad (1)$$

If we denote the Fourier transform of the shape function by $f(\tau)$, we can easily find that

$$f(\tau)=\sum_{n=0}^{\infty}\frac{(i\tau)^n}{n!}\langle\omega^n\rangle_{AV}. \qquad (2)$$

If we are concerned with electric or magnetic dipole radiation linearly polarized parallel to the x-axis, the intensity of radiation, emitted or absorbed, accompanied by the transition $a\to b$ is proportional to $|\mu_{x,ab}|^2$, μ_x being the x-component of the electric or magnetic dipole moment of the system which we are interested in. Thus we have for $\langle\omega^n\rangle_{AV}$

$$\langle\omega^n\rangle_{AV}=\sum_{a,b}\omega_{a,b}^n\,|\mu_{x,ab}|^2/\sum_{a,b}|\mu_{x,ab}|^2. \qquad (3)$$

where ω_{ab} is the circular frequency corresponding to the transition $a\to b$. This expression is just the starting point of Van Vleck's method of moment.

Now, we take the Heisenberg representation for the matrix μ_x. Then it is easy to see that

$$\langle\omega^n\rangle_{AV}=i^{-n}T_r.[d^n\mu_x(t)/dt^n\cdot\mu_x(t)]/T_r.[\mu_x^2(t)]. \qquad (4)$$

Inserting this into Eq. (2), we have a very simple expression for the Fourier transform $f(\tau)$:

$$f(\tau)=T_r.[\mu_x(t+\tau)\mu_x(t)]/T_r.[\mu_x(t)\mu_x(t)]. \qquad (5)$$

As the trace of the matrix for an observable is proportional to the mean value of it, we see that the Fourier transform of the shape function is nothing other than the auto-correlation function of the dipole moment, as it is the case in the classical theory.[5)]

The matrix $\mu_x(t+\tau)$ can be derived from the matrix $\mu_x(t)$ by the unitary transformation

$$\mu_x(t+\tau)=\exp(iH\tau/\hbar)\,\mu_x(t)\exp(-iH\tau/\hbar), \qquad (6)$$

where H is the Hamiltonian of the system. We now divide the Hamiltonian H into the two constituents H_0 and H_1:

$$H=H_0+H_1.$$

where H_0 is the part of the Hamiltonian, with the transition between the eigenstates of which we identify the spectral line, and H_1 is the interaction between dipoles which gives rise to the line width.

If we take the representation in which H_0 is diagonal, then the matrix element $(j|\mu_x(t+\tau)|k)$ corresponding to the transition from the eigenstate j of H_0 with energy $E_{0,j}$ to the eigenstate k with energy $E_{0,k}$ becomes

$$(j|\mu_x(t+\tau)|k)=\exp(i\omega_{0,jk}\tau)\cdot(j|\exp(iH_1\tau/\hbar)\mu_x(t)\exp(-iH_1\tau/\hbar)|k), \qquad (7)$$

where

$$\omega_{0,jk}=(E_{0,j}-E_{0,k})/\hbar.$$

Inserting this expression into Eq. (5) and inversely transforming from $f(\tau)$ to $g(\omega)$, we obtain as the shape function $g_{jk}(\omega)$ corresponding to the transition $j\to k$

$$g_{jk}(\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\exp[-i(\omega-\omega_{0,jk})\tau]\times(j|\exp(iH_1\tau/\hbar)\mu_x(t)\exp(-iH_1\tau/\hbar)|k)\times(k|\mu_x(t)|j)d\tau/|(j|\mu_x(t)|k)|^2. \qquad (8)$$

Eq. (6) is valid, in the adiabatic approximation, even when H_1 contains the time explicitly, as in the theory of pressure broadening, if we substitute the product $H_1\tau$ by the integral $\int_t^{t+\tau} H_1(t')dt'$. When this substitution is made, Eq. (8) is just the standard form of the line shape function in the Fourier transform theory of the pressure broadening. In any case, we see that the problem of line shape can be reduced to the Fourier analysis of the interaction representation for the dipole moment.

1) J. H. Van Vleck, Phys. Rev. **74** (1948), 1168.
2) H. M. Foley, Phys. Rev. **69** (1946), 616.
3) P. W. Anderson, Phys. Rev. **76** (1949), 647.
4) M. Mizushima, Phys. Rev. **83** (1951), 94.
5) M. C. Wang and G. E. Uhlenbeck, Rev. Mod. Phys. **17** (1945), 323.

Non-local Field and Non-local Interaction

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Though the non local field theory proposed by Yukawa[1] has many interesting aspects, this theory seems to us to be not so powerful for the divergence difficulties.[2] It is very doubtful whether the method of Feldman, Yang and Källen can be extended to the non-local theory. Further there is no reason for the perturbation treatment is applicable in this theory. Therefore the circumstance seems to be not so good for its future development.

Apart from these problems, using the traditional method, Kristensen[3] and Møller have recently shown that there is a possibility of removing the divergences by introducing the suitable form factor from the only non-local interaction. This fact is very suggestive for us. As already Tokuoka and the author[4] have indicated, if we construct the associated local Lagrangian from the non-local one, it is possible to transform the non-local field to the non-local interaction. The purpose of this letter is to give the relations between these two theories and then to pursuite the possibilities of the generalization of the non local-field theory from standpoint the of the convergence problem.

According to the previous letter[4], we define the associated local Lagrangean L from the non-local Lagrangean $\mathfrak{L}$

$$L(x)=\int dr\left(x+\frac{r}{2}|\mathfrak{L}|x-\frac{r}{2}\right), \quad (1)$$

and take the interaction Lagrangean for the non local field

$$\mathfrak{L}=gU^*VU, \quad (2)$$

and the Fourier expansions of non-local fields

$$\left(X+\frac{r}{2}|A^i|X-\frac{r}{2}\right)$$

$$=\frac{1}{(2\pi)^4}\int dl^i e^{-il^iX}a^i(l^i)F^i(r,l^i), \quad (3)$$

where $A^1=U^*$, $A^2=V$ and $A^3=U$. Then we have

$$\bar{L}=\int dx L(x)$$

$$=\frac{g}{(2\pi)^{12}}\int dx\int dl^1dl^2dl^3E(l^1,l^3)$$

$$\times e^{-i\sum_i l^i x}u^*(-l^1)v(l^2)u(l^3) \quad (4)$$

and

$$E(l',l^3)=\int dr_1F^1(r_1,-l^1)e^{-i\frac{l^1}{2}r_1}$$

$$\times\int dr_2F^2(r_2,-l^1-l^3)\ e^{-i\frac{l^1-l^3}{2}r_2}$$

$$\times\int dr_3F^3(r_3,l^3)e^{i\frac{l^3}{2}r_2}. \quad (5)$$

As shown by Kristensen and Møller, if we assume that the integral which appears in the equation (5)

$$\int dr\ F^i(r,-L)e^{-ilr}=G^i(L,l) \quad (6)$$

depends only on the variable

$$ll^2=l^2-\frac{(lL)^2}{L^2} \quad (6')$$

and $\lim_{ll\to 0}G(ll)=1$, the equation (5) becomes

$$E(l^1,l^3)=G^2\left(l^1+l^3,\ \frac{1}{2}(l^1-l^3)\right) \quad (7)$$

which agrees with the result of Møller's theory. Therefore, we have the relations, between the two

theories by (6) and (6′).

For the sake of the fact that (6) must depend only on the variable (6′), we can conclude that F must be

$$F(r, -L)=\sqrt{-L^2}\,\delta(rL)f(r^2) \quad (8)$$

and the relation between $f(r^2)$ and $G(\Pi)$ is

$$G(\Pi)=\frac{2\pi}{\Pi}\int_0^\infty dr^2 f(r^2)\sin(\Pi^2 r^2)^{\frac{1}{2}}. \quad (9)$$

According to Yukawa theory, we have $f(r^2)=\frac{1}{2\pi\lambda}\delta(r^2-\lambda^2)$ and then $G(\Pi)=\sin\lambda\Pi/\lambda\Pi$. This is too weak to remove the divergences.

Consequently, we have the following properties for $f(r^2)$ so as to remove the divergences through the relation with $G(\Pi)$:

i) $f(r^2)$ should not be only δ function type.

ii) If $f(r^2)$ would have poles, it should be forbidden that $f(r^2)$ has the poles at the positive values of r^2.

iii) Although $f(r^2)$ would have no poles, $f(r^2)$ should become zero sufficient strongly as $r^2\to\infty$.

The above conditions seem to be not so useful to determine the function $f(r^2)$, but will be very suggestive to expect the future extension. At this present, we can only conclude that the cut-off factor $G(\Pi)$ which are deduced from $f(r^2)$ will converge as $e^{-\lambda\Pi}$ or $e^{-\lambda^2\Pi^2}$ or more strongly.

We have no guiding principle to construct $f(r^2)$, such as the reciprocity which has played the very important role in Yukawa theory. However, in order to develope the theory, it is desirable to find the new principle and this principle will have to introduce the above mentioned properties for $f(r^2)$. Full account will appear in this journal.

1) H. Yukawa, Phys. Rev. **77** (1950), 219; **80** (1950), 1047.

2) D. Yennie, Phys. Rev. **80** (1950), 1053; J. Rayski, Proc. Roy. Soc. A **206** (1951), 575.

3) P. Kristensen and C. Møller, Det. Kgl. Danske Vidensk. Selsk. Mat. Fys. Medd. in press.

4) Z. Tokuoka and Y. Katayama, Prog. Theor. Phys. **5** (1951), 132.

Note on Invariancy of Some Fundamental Equations of Physics

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Theory of relativity has developed in close connection with continuous group of transformations, e g., the special relativity with the Lorentz group L, the general relativity with the group G of general transformations, unified theories with G or its enlarged groups, etc. Recently Ueno and Takeno studied the problem of equivalent observers by using the theory of continuous groups[1]. From the same standpoint a relativistic theory of uniformly accelerated motions and that of rotating disk were constructed by Hill[2] and Takeno[3] respectively. Further Hill tried to look for the enlargement of L from kinematic considerations.[4]

There exists a close relation between a continuous group of transformations and the equations of physics which are invariant under that group. Concerning the study of this relation it seems that there exist three methods; (I) to obtain equations from a given group, conversely (II) to obtain groups from a given equations, further (III) to research groups and equations simultaneously in some way.[1] By the method of (I) Dirac obtained wave equations which are invariant under the group of motions of de Sitter space-time and the conformal group C of Minkowski space-time respectively.[5] In this letter, by the method of (II), we shall research continuous groups of transformations which leave some given physical equations invariant.

A law of physics is generally expressed by a set of functional relations

$$F_p(x^i, A, B, \cdots; \partial A/\partial x^i, \cdots; \partial^2 A/\partial x^i \partial x^j, \cdots)=0 \quad (1)$$

$$(x^i=(x, y, z, ct),\ p=1, \cdots, n)$$

between physical quantities A, B, $\cdots$ and their derivatives of required orders. The invariancy of (1) under a transformation: $'x^i='x^i(x)$ means that the same functional relations between transformed quantities

$$F_p('x^i, 'A, 'B, \cdots; \partial' A/\partial' x^i, \cdots; \partial^{2'} A/\partial' x^i \partial' x^j, \cdots)=0 \quad (1')$$

follows from (1).[6] In special relativity transformation laws of physical quantities are defined for L. We assume that these transformation laws hold good also for general transformations; for example, if a physical quantity transforms as a covariant vector under general transformations.

In the following we shall obtain transformations which leave some given equations of physics invariant. As all such transformations form a continuous group, we have used the theory of the infinitesimal transformations of a group in getting the following results.

In special relativity the propagation of light is usually expressed by

$$\eta_{ij}dx^i dx^j=0,\ (-\eta_{\alpha\alpha}=\eta_{44}=1,\ \text{other}\ \eta_{ij}=0,\ \alpha=1,2,3) \tag{2}$$

or $$\Box\varphi\equiv\eta^{ij}\partial^2\varphi/\partial x^i\partial x^j=0,\ (\eta_{ik}\eta^{jk}=\delta^{ij}). \tag{3}$$

The group of transformations leaving (2) invariant is C, which consists of L (including rotations in the ordinary space), the group T of translations and the group D of dilatations of Minkowski space-time and an Abelian group P of four parameters. P was obtained by Page from a kinematic standpoint and its transformations lead to uniformly accelerated reference systems in his sense.[7] The infinitesimal transformation of P was already obtained by Mimura and Iwatsuki.[8] On the other hand the group of transformations leaving (3) invariant consists of L, T and D, and is different from the one which leaves (2) invariant. This discrepancy disappears if we consider the rectilinear motion of light in addition to (2).

Next the group of transformations which leave the equations for 4-potential

$$\Box\varphi^i=s^i \tag{4}$$

invariant consists of L and T or L, T and D according as the source s^i exists or not. The group of transformations which leave Maxwell equations

$$\partial F^{ij}/\partial x^j=s^i,\ \epsilon^{ijkl}\partial F_{jk}/\partial x^l=0,\ (F_{(ij)}=F^{(ij)}=0) \tag{5}$$

invariant is characterized by $\partial\xi^i/\partial x^i=\text{const.}$, where ξ^i is the vector of an infinitesimal transformation. It is to be noted that (5) is obtained by generalizing the ordinary Maxwell equations only in a formal manner. The electromagnetic field is expressed by a contravariant tensor F^{ij} in the equation of (5) and by a covariant tensor F_{ij} in the second. As we have no definite method to raise and lower the indices of a tensor, we have no choice but to regard these two tensors as separate expressions of the same field. And consequently, the two groups of transformations which leave (4) and (5) invariant respectively are not identical. Only in the special relativistic frame these two tensors are connected by $F_{ij}\eta^{ik}\eta^{jl}=F^{kl}$ and the above two groups become identical.

In the same way we can consider about the wave equations of meson (scalar or vector)

$$(\Box+\varkappa^2)\phi=0\quad\text{or}\quad(\Box+\varkappa^2)\phi_i=0, \tag{6}$$

$$\left.\begin{aligned}&\text{and}\ \partial\phi/\partial x^i=\varkappa\phi_i,\quad\partial\phi^i/\partial x^i=\varkappa\phi\\&\text{or}\quad\partial\phi^j/\partial x^i-\partial\phi^i/\partial x^j=\varkappa\chi_{ij},\partial\chi^{ij}/\partial x^j=\varkappa\phi^i.\end{aligned}\right\} \tag{7}$$

The group of transformations which leave (6) or (7) invariant is composed of L and T or characterized by $\partial\xi^i/\partial x^i=0$ respectively.

The group of transformations which leave Dirac equation

$$\{\gamma^i(\partial_i+\varphi_i)-\varkappa\}\psi=0,\quad(\gamma^i\gamma^j-\eta^{ij}) \tag{8}$$

invariant consists of L and T. We can prove this without using infinitesimal transformations.

Thus we can see that it is almost impossible to enlarge L without deforming various equations which are used in the special relativistic frame.

1) Y. Ueno and H. Takeno, Prog. Theor. Phys. in press.
2) E. L. Hill. Phys. Rev. **67** (1945), 358.
3) H. Takeno, Prog. Theor. Phys. **7** (1952), 367.
4) E. L. Hill, Phys. Rev. **84** (1951), 1165.
5) P. A. M. Dirac, Ann. of Math. **36** (1935), 657; **37** (1936), 429.
6) This definition is somewhat different from that in general relativity.
7) L. Page, Phys. Rev. **49** (1936), 254.
8) Y. Mimura and T. Iwatsuki, Journ. Sci. Hiroshima Univ. **1** (1931), 111. The finite transformation is already known, too. See, for example, H. T. Engstrom and M. Zorn. Phys. Rev. **49** (1936), 701.

Linear Meson Wave Equation in de Sitter Space

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Dirac[1] has given

$$\{a_\mu a_\nu m_{\mu\nu} - 2Rm\}\psi = 0, \tag{0.1}$$

as the linear wave equation for the electron in de Sitter space of radius R. Here $m_{\mu\nu}$ are given by

$$m_{\mu\nu} = x_\mu p_\nu - x_\nu p_\mu = -i\hbar\left(x_\mu \frac{\partial}{\partial x_\nu} - x_\nu \frac{\partial}{\partial x_\mu}\right), \tag{0.2}$$

and satisfy the commutation rule

$$[m_{\mu\nu}, m_{\lambda\kappa}] = m_{\mu\nu}m_{\lambda\kappa} - m_{\lambda\kappa}m_{\mu\nu}$$
$$= \delta_{\mu\lambda}m_{\nu\kappa} - \delta_{\mu\kappa}m_{\nu\lambda} + \delta_{\nu\kappa}m_{\mu\lambda} - \delta_{\nu\lambda}m_{\mu\kappa}. \tag{0.3}$$

We shall show, proceeding analogously, that the linear wave equation for the meson in de Sitter space

$$\{S_{\mu\nu}m_{\mu\nu} - 2Rm\}\psi = 0, \tag{1.1}$$

where the spin operator $S_{\mu\nu}$ is given by

$$S_{\mu\nu} = \beta_\mu\beta_\nu - \beta_\nu\beta_\mu, \tag{1.2}$$

the β_μ is being matrices satisfying the Duffin-Kemmer[2] commutation relations

$$\beta_\mu\beta_\nu\beta_\lambda + \beta_\lambda\beta_\nu\beta_\mu = \delta_{\mu\nu}\beta_\lambda + \delta_{\nu\lambda}\beta_\mu. \tag{1.3}$$

From this we shall determine the current-charge density, the momentum-energy density and the constant of motion giving the spin momenta. Finally the second order wave equation will be derived.

We note that near the point (0, 0, 0, 0, R), the equation (1,1) reduces on division by R to

$$\beta_5\beta_i p_i\psi - \beta_i\beta_5 p_i\psi - m\psi = 0 \quad (i = 1, \cdots, 4)$$

Multiplying on the left by $\beta_f\beta_5$, where f is a fixed index, arbitrarily chosen from 1,$\cdots$, 4, we get

$$\beta_f\beta_5\beta_5\beta_i p_i\psi - \beta_f\beta_5 m\psi = 0, \tag{1.4}$$

since by (1.3), $\beta_f\beta_5\beta_i\beta_5 = 0$. As the β_μ's satisfy (1.3), we see that

$$\beta_f\beta_5\beta_5\beta_i\beta_f\beta_5\beta_5\beta_j\beta_f\beta_5\beta_5\beta_k$$
$$+ \beta_f\beta_5\beta_5\beta_k\beta_f\beta_5\beta_5\beta_j\beta_f\beta_5\beta_5\beta_i$$
$$= \delta_{fi}\delta_{fi}\beta_f\beta_5\beta_5\beta_k + \delta_{fi}\delta_{fk}\beta_f\beta_5\beta_5\beta_i. \tag{1.5}$$

It follows that the commutation relations for the $\beta_f\beta_5\beta_5\beta_i$'s are the same as those for the β_i's in Minkwowskian space. This establishes (1.1).

The Hermitian conjugate equation to (1.1) is

$$\psi^+\{S_{\mu\nu}m_{\mu\nu} - 2Rm\} = 0, \tag{1.6}$$

where

$$\overleftarrow{m}_{\mu\nu} = x_\mu \overleftarrow{p}_\nu - x_\nu \overleftarrow{p}_\mu = i\hbar\left(x_\mu \frac{\partial}{\partial x_\nu} - x_\nu \frac{\partial}{\partial x_\mu}\right), \tag{1.7}$$

since $\overleftarrow{p}_\mu = i\hbar\dfrac{\partial}{\partial x_\mu}$.

The current-charge density ρ_ν is obtained as usual by multiplying (1.1) by ψ^+ on the left, multiplying (1.6) by ψ on the right, and subtracting the former from the latter. Thus

$$i\hbar\frac{\partial}{\partial x_\nu}\psi^+ S_{\mu\nu}x_\mu\psi - i\hbar\frac{\partial}{\partial x_\mu}\psi^+ S_{\mu\nu}x_\nu\psi = 0,$$

or interchanging the indices μ, ν in the second term, we get

$$\frac{\partial\rho_\nu}{\partial x_\nu} = 0, \text{ where, } \rho_\nu = 2\psi^+ S_{\mu\nu}x_\mu\psi. \tag{2 1, 2 2}$$

Since $x_\mu x_\nu = 0$, it follows that $x_\nu\rho_\nu = 0$, that is, the vector ρ_ν lies in the de Sitter space.

The momentum-energy density tensor $T_{\nu\lambda}$ is obtained in similar fashion by multiplying (1.1) by $\psi^+\overrightarrow{m}_{\mu\lambda}$ from the left, multiplying (1.6) by $\overrightarrow{m}_{\mu\lambda}\psi$ from the right, and substracting the first result from the second. Thus

$$i\hbar\psi^+\left\{S_{\mu\nu}\overrightarrow{m}_{\mu\lambda}x_\mu\frac{\partial}{\partial x_\nu}\right\}\psi - i\hbar\,\psi^+\left\{S_{\mu\nu}\overrightarrow{m}_{\nu\lambda}x_\mu\frac{\partial}{\partial x_\nu}\right\}\psi$$
$$+ i\hbar\frac{\partial\psi^+}{\partial x_\nu}\{S_{\mu\nu}\overrightarrow{m}_{\mu\lambda}x_\mu\}\psi - i\hbar\psi^+\left\{S_{\mu\nu}\overrightarrow{m}_{\mu\lambda}x_\nu\frac{\partial}{\partial x_\mu}\right\}\psi$$
$$= 0.$$

Applying (1.7) to the last term, we get, after cancellation of the second and fourth terms,

$$i\hbar\frac{\partial}{\partial x_\nu}\{\psi^+ S_{\mu\nu}\overrightarrow{m}_{\mu\lambda}x_\mu\psi\} = 0, \tag{2.3}$$

so that

$$T_{\nu\lambda} = \psi^+ S_{\mu\nu}m_{\mu\lambda}x_\mu\psi. \tag{2.4}$$

An operator C will be a constant of motion if it commutes with the operator H in the wave equation. We may compute $[m_{\mu\nu}, H]$ from the relations

$$H = \sum_\nu \sum_{\mu>\nu} S_{\mu\nu}m_{\mu\nu} - 2Rm, \tag{3.0}$$

and (0.3); and $[S_{\mu\nu}, H]$ from (3.0) and (1.2). We would then get

$$[m_{\mu\nu}-S_{\mu\nu},\ H]=[m_{\mu\nu}-S_{\mu\nu},\ S_{\nu\mu}m_{\mu\nu}-2Rm]=0 \tag{3.1}$$

Hence

$$C=m_{\mu\nu}-S_{\mu\nu}, \tag{3.2}$$

are the constants of motion. It follows that $S_{\mu\nu}$ given by (1.2) are the spin momenta. Of these, the S_{i5}'s are the spin linear momenta, as has been observed by Dirac.

The linear wave equation for elementary particles of higher spin can be obtained as follows. We determine (cf. (1.2)) suitable expressions for the spin operator $S_{\mu\nu}$ in terms of spin matrices β_μ, obeying suitable commutation relations (cf. (1.3)), and substitute these expressions in (1.1). The second order wave equation is obtained by eliminating the matrices β_μ's from the linear wave equation by a method used by Kemmer. Thus multiplying the equation by $S_{\mu\nu}S_{\mu\nu}m_{\mu\nu}m_{\mu\nu}$ and expanding the brackets, we get, using (1.3), (1.2), (1.1)

$$\{\beta_\mu\beta_\nu\beta_\nu\beta_\mu\beta_\mu\beta_\nu-\beta_\nu\beta_\mu\beta_\mu\beta_\nu\beta_\nu\beta_\mu\}m_{\mu\nu}m_{\mu\nu}m_{\mu\nu}\psi$$
$$-SR^3m^3\psi=0,$$

or

$$\{\beta_\mu\beta_\nu\beta_\nu(-\beta_\nu\beta_\mu\beta_\mu+\delta_{\nu\mu}\beta_\mu+\delta_{\mu\mu}\beta_\nu)$$
$$-\beta_\nu\beta_\mu\beta_\mu(-\beta_\mu\beta_\nu\beta_\nu+\delta_{\mu\nu}\beta_\nu+\delta_{\nu\nu}\beta_\mu)\}m_{\mu\nu}m_{\mu\nu}m_{\mu\nu}\psi$$
$$-8R^3m^3\psi=0.$$

Hence the second order wave equation is

$$\{m_{\mu\nu}m_{\mu\nu}+4R^2m^2\}\psi=0. \tag{4.0}$$

1) Dirac, Ann. of Math. **36** (1935), 657.
2) Kemmer, Proc. Roy. Soc. Lond. **A 173** (1939), 92.

On Yukawa's Theory of Non-local Field

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September 30, 1952

In previous papers,[1)2)] we remarked that the equations of motion and the commutation relation of the non-local field proposed by Yukawa[3)] can be deduced from those of the ordinary local field by a suitable canonical transformation in the case of no interaction. We also conjectured the equivalence of the non-local fields to that of the local fields[1)] by exhibiting that the self-energy of a local charged spinor particle due to a non-local neutral scalar field diverges in the same manner as that due to a local neutral scalar field. Yukawa[4)] pointed out that our conjecture is based on rather a special example in which the non-local field appears only linearly in the interaction Lagrangian density, and so the investigation into the interaction of two non-local fields would reveal the characteristic features of his theory.

According to this suggestion, we calculated the self-energy of a non-local charged scalar particle due to a non-local neutral scalar field. Assuming the interaction Lagrangian as

$$f(U^*IU), \tag{1}$$

where U, U^* and V mean the non-local charged scalar field, its Hermite conjugate, and the non-local neutral field respectively, and substituting (1) into the S matrix given by Yukawa[5)], the self-energy can be calculated following the ordinary procedure. The result was, however, exactly the same as before in contradiction to Yukawa's anticipation. The reason is considered as follows. The commutation relation of the non-local field is given by

$$[U^*(x_\mu, r_\mu), U(x'_\mu, r'_\mu)]$$
$$=-\int\frac{k_4}{|k_4|}\delta(k_\mu{}^2+\varkappa^2)\delta(k_\mu-k'_\mu)\delta(r_\mu{}^2-\lambda^2)\delta(k_\mu r^\mu)$$
$$\times\delta(r_\mu-r'_\mu)e^{ik_\mu(x^\mu-x^{\mu\prime})}\,(dk_\mu). \tag{2}$$

The appearance of $\delta(r_\mu-r'_\mu)$ means that the interactions take place only if $r_\mu=r'_\mu$. Therefore, every part of a non-local particle interacts with the part of other non-local particle for which the internal coordinate are the same (see figure). Thus we can

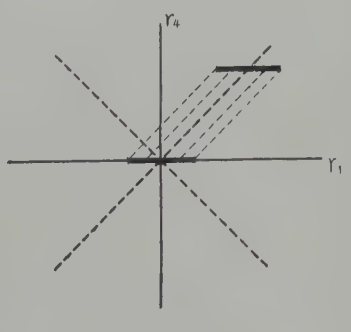

Fig. 1.

not expect the averaging out of the high frequency part of the intermediating waves notwithstanding the introduction of a finite extension for the particle. The term $\delta(r_\mu - r'_\mu)$ played also a decisive role in deducing the commutation relation (2) from that of the local field by a canonical transformation. Thus above result may be interpreted as showing that the non-local field which is characterized by the commutation relation (2), and which was proposed by Yukawa as an example of his general considerations, is an equivalent dynamical system to the ordinary local field, and is too simple to express the essential features of the non-local field. Other type of non-local fields, for example, the one proposed by Yennie[6] or Rayski[7], avoid this difficulty by modifying the commutation relation to

$$[U^*(x_\mu, r_\mu), U(x'_\mu, r'_\mu)]$$

$$= -\int_{|k_4|}^{k_4} \delta(k_\mu{}^2 + \varkappa^2)\,\delta(k_\mu - k'_\mu)\,\delta(r_\mu{}^2 - \lambda^2)\,\delta(k_\mu r^\mu)$$

$$\times \delta(r'_\mu{}^2 - \lambda^2)\,\delta(k'_\mu r'^\mu)\, e^{ik_\mu(x^\mu - x'^\mu)}\,(dk_\mu).$$

The difficulty of the Yukawa's theory can be avoided by this modification, and a relativistically invariant cut off factor appears as the result of introducing a finite extension for the particle. But their method lacks necessity in the way of the modification, and further investigations seem to be indispensable for the ultimate solution of the problem.

With all these unsatisfactory features in the present form, however, the concept of the non-local field seems very interesting to us. First it is in connection with the non-local interation. Recently Sakata[8] and others classified the interactions into the first kind for which the renormalization method can be performed in a closed form, and the second for which this is not the case. The interactions of the second kind necessarily lead to non-local interactions. For the system with non-local interactions, however, Hamiltonian formalism fails, and it seems quite dubious whether the traditional local theory can be adapted to include them. The second view point is connected to the mass spectrum of elementary particles. Nambu[9] pointed out that the mass of elementary particles measured in unit of $137\times$ (electron mass) take integer or half integer values. The existence of such a simple regularity between the mass suggests strongly the notion of "Urmaterie". It implies that the present elementary particles corresponds to various energy states of the internal motion of this Urmaterie, and in this respect it seems likely that the field that describes the Urmaterie is nothing but the non-local field.

We wish to express our sincere gratitude to Prof. S. Sakata for his continual encouragement and criticism. We also thank Prof. H. Yukawa for giving us an opportunity of discussing on this subject during his stay in Japan in the summer of 1952.

Detailed paper will be published in a soon later issue of this journal.

1) O. Hara and H. Shimazu, Prog. Theor Phys. **5** (1950), 1055.
2) O. Hara and H. Shimazu, Prog. Theor. Phys. **7** (1952), 255.
3) H. Yukawa, Phys. Rev. **77** (1950), 219.
4) H. Yukawa, Prog. Theor. Phys. **6** (1951), 133.
5) H. Yukawa, Phys. Rev. **80** (1950), 1047.
6) D. R. Yennie, Phys. Rev. **80** (1950), 1053.
7) J. Rayski, Proc. Roy. Soc. **A206** (1951), 575.
8) S. Sakata, H. Umezawa and S. Kamefuchi, Prog. Theor. Phys. **7** (1952), 377.
9) Y. Nambu, Prog. Theor. Phys. **7** (1952), 595.

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Interaction of π-Electrons in the Acetylene Molecule*

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The acetylene molecule has been treated as a system of four π-electrons, and its lower excited energy levels have been calculated using both MO method with configuration interaction and the HL method including ionic-homopolar resonance. The Slater $2p\pi$ atomic orbitals with effective charge 3.18 have been used in each calculation. The results show that the effects of configuration interaction in the MO case or of resonance in the HL case on the energy levels are fairly large, amounting to several electron volts. It is found that the lower "vertical" excitation energies from the $^1\Sigma_g^+$ ground state are 4.88 eV ($^3\Sigma_u^+$), 6.27 eV ($^3\Delta_u$) and 7.59 eV ($^3\Sigma_u^-$, $^1\Sigma_u^-$), and so on. The effects of the configuration interaction and of the ionic-homopolar resonance are discussed in connection with the interrelation between the MO wave functions and the HL ones.

§ 1. Introduction

The lower excited levels of unsaturated hydrocarbon molecules have been extensively studied by the atomic or molecular orbital method. The molecules treated thus far are, however, confined almost to those with double bonds. In the present paper we investigate the acetylene molecule, which has a carbon-carbon triple bond. For the purpose of calculating the lower excited levels, we treat this molecule*** as a system of four π-electrons, in which the effect of the other electrons is represented by a suitable potential acting on the π-electrons. This approximation,**** although open to some questions,[1)7)] has been used so far in many investigations on unsaturated hydrocarbon molecules with considerable success,[2)-7)] and simplifies the "model" to such an extent as to allow us to make considerably refined calculations described in the following.

Now, Craig, Coulson and others[4)-7)] have recently shown that the inclusion of configuration interaction in a MO (molecular orbital) calculation of this sort is indispensable for

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* A preliminary report on this research was given by one of the authors (M.K.) at the conference on "Quantum Mechanical Methods in Valence Theory" held at Shelter Island, U.S.A., 1951.

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*** Our present calculation can be extended to the polyacetylene compounds; the calculation relating to the diacetylene molecule is now in progress in our laboratory.

**** What is called the Hueckel approximation (cf. Ref. 1.).

obtaining a correct prediction of the excited energy levels. From the viewpoint of the HL (Heitler-London) theory, this is equivalent to the inclusion of the resonance among various homopolar and ionic structures, or ionic-homopolar resonance. However, the full inclusion of CI (configuration interaction) or IHR (ionic-homopolar resonance) leads to very (or sometimes prohibitively) troublesome calculations for complicated molecules. Thus it is desirable to perform these detailed calculations for simpler molecules, and hereby to study the criteria for the economical selection of important configurations or structures.[7] Our investigation on the acetylene molecule has been made also with these views in mind.

In the present investigation, the calculation of the energy levels is made by the MO method with CI (Section 3)* in the first place, and then the same problem is examined from the standpoint of the HL method with IHR (Section 4). As is well known, the MO method and the HL method merge into one[8], if the effects of CI in the former and those of IHR in the latter are fully included. Thus it is evident that our HL calculation must lead to the same results as obtained by the MO method with CI. However, the approach to the final results by the HL method is interesting, since we can make a HL wave function correspond to a chemical structure formula of a molecule.

These results will be discussed in Section 5 of this paper. Especially the interrelation between the MO and HL treatments will be examined there, as well as the significance of the simpler approximations, e.g., the single configuration (or structure) approximation.

§ 2. π-orbitals and Hamiltonian for acetylene

As mentioned in the introduction, the acetylene molecule is treated as a 4-electron system, these four electrons being those of the four $2p\pi$ orbitals of the carbon atoms. For the treatment of the axially symmetric acetylene molecule, it is advantageous to use the complex $2p\pi$ atomic orbital functions rather than the real ones,** the former having an axially symmetric charge distribution and the latter a marked directional property around the molecular axis. Thus the $2p\pi$ functions are written for one carbon atom as :***

$$a_{\pm}(q)=(\delta^5/2\pi)^{1/2}r_{aq}\exp(-\delta r_{aq})\sin\theta_{aq}\exp(\pm\varphi_q i), \tag{1}$$

and for the other carbon atom as :

$$b_{\pm}(q)=(\delta^5/2\pi)^{1/2}r_{bq}\exp(-\delta r_{bq})\sin\theta_{bq}\exp(\pm\varphi_q i). \tag{1'}$$

Here the polar coordinates r, θ and φ are defined as seen in Fig. 1, and $2\delta=3.18$ is effective charge for the carbon $2p\pi$ orbitals[3)9)].

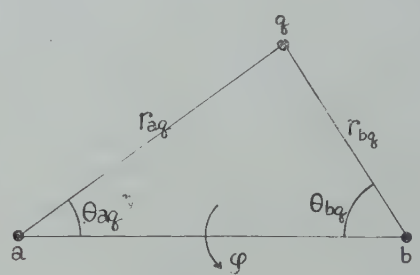

Fig. 1.

* In his private letter, Dr. I. G. Ross in London told one of us (M.K.) that he had finished a calculation of the acetylene excited levels by the MO method with CI (to be published in *Trans. Faraday Soc.*).

** See, however, Section 5.

*** In the formulae in the present paper, the atomic units (a. u.) are used, the units of energy and length being 27.204 eV and 0.529A respectively.

The hamiltonian for the molecule is formulated as :

$$\boldsymbol{H}=\sum_q\left(-\frac{1}{2}\Delta_q+U_q\right)+\sum_{p<q}(1/r_{pq}),\quad (p,\,q=1,\cdots 4), \tag{2}$$

where U_q denotes the potential acting on the q-th electron due to the nuclei and the core electrons, i.e., the electrons other than those occupying the $2p\pi$ orbitals. The explicit expression for U_q can be obtained under the following simplifying assumptions :

i) The exchange interactions of the $2p\pi$ electrons with the core electrons may be neglected.

ii) The $1s$ electrons of C and H atoms completely screen their own nuclei, i.e., the effect of each of these electrons may be represented by reducing the charge of each nucleus by $+e$ ($+e$=protonic charge).

iii) The contributions to U_q of the electrons in $2s$-$2p\sigma$ hybridized orbitals of the carbon atoms are equated to the sum of the electrostatic potentials due to these electrons in the isolated atoms.

Thus we may write as follows :

$$U_q=u_{aq}+u_{bq};$$

$$u_{aq}=-(4/r_{aq})+\int(1/r_{jq})[|a_{2s}(j)|^2+|a_{2p\sigma}(j)|^2]\,d\tau_j, \tag{3}$$

and a similar expression for u_{bq},

where a_{2s} and $a_{2p\sigma}$ denote the $2s$ and $2p\sigma$ orbitals of the carbon atom a.

The above expression for U_q is essentially the same as that used by Goeppert-Mayer and Sklar[3], but further refinements may be possible especially by adding to U_q an integral operator describing the exchange interaction with the core electrons, and also by calculating the charge distribution of the core electrons which is not simply the superposition of atomic ones on account of the overlapping of orbitals belonging to different atoms. These refinements will, however, be reserved for another paper.

The carbon-carbon internuclear distance in the acetylene molecule is taken to be 1.20A.[10]

§ 3. Calculation by MO method

In this section we calculate the energy levels of the acetylene molecule by the MO method with CI. The four linear independent LCAO molecular orbitals for the π-electrons appropriate to the symmetry $D_{\infty h}$ of the molecule are made of the atomic orbitals a_+, a_-, b_+ and b_- :

$$\begin{aligned} u_+&=(2N_u)^{-1/2}(a_++b_+), & u_-&=(2N_u)^{-1/2}(a_-+b_-),\\ g_+&=(2N_g)^{-1/2}(a_+-b_+), & g_-&=(2N_g)^{-1/2}(a_--b_-), \end{aligned} \tag{4}$$

where

$$N_u=1+S,\qquad N_g=1-S,$$

and

$$S=\int a_\pm^*(j)\,b_\pm(j)\,d\tau_j\ \text{(overlap integral)}. \tag{5}$$

It is readily seen that the symmetry of u_+ and u_- is Π_u, and that of g_+ and g_- Π_g. The orbital energies ε_u and ε_g are determined by $u_\pm$ and $g_\pm$ respectively, as follows :

$$\varepsilon_u=\int u_\pm^*(j)\left(-\frac{1}{2}\Delta_j+U_j\right)u_\pm(j)\,d\tau_j=N_u^{-1}(I+F),$$
$$\varepsilon_g=\int g_\pm^*(j)\left(-\frac{1}{2}\Delta_j+U_j\right)g_\pm(j)\,d\tau_j=N_g^{-1}(I-F), \tag{6}$$

where

$$I=\int a_\pm^*(j)\left(-\frac{1}{2}\Delta_j+U_j\right)a_\pm(j)\,d\tau_j,$$
$$F=\int b_\pm^*(j)\left(-\frac{1}{2}\Delta_j+U_j\right)a_\pm(j)\,d\tau_j. \tag{7}$$

For the evaluation of the integrals I and F, we make use of the (approximate) relation :[3]

$$\left[-\frac{1}{2}\Delta_q+u_{aq}+\int(1/r_{jq})\,|a_\mp(j)|^2 d\tau_j\right]a_\pm(q)=E_{2p}\,a_\pm(q), \tag{8}$$

where E_{2p} is the orbital energy of a $2p$ electron in a carbon atom in the valence state. Thus, as a result of the numerical computation explained in Appendix, we have

$$\varepsilon_u=E_{2p}-40.05\text{ eV},\quad \varepsilon_g=\varepsilon_u+8.05\text{ eV}, \tag{9}$$

which shows that the orbitals u_+ and u_- are more stable.

Taking into account the ground state configuration $(u_\pm)^4$ as well as all the excited state configurations $(u_\pm)^3(g_\pm),\cdots,(g_\pm)^4$, we can construct the ASMO (antisymmetrized molecular orbital) wave functions X_i of various symmetries and multiplicities in the usual manner[3]. The result is listed in Table 1, in which the following abbreviation is used :

$$(\text{abcd};\,\chi_i)=(4!)^{-1/2}\sum_P(-1)^P\boldsymbol{P}\,a(1)b(2)c(3)d(4)\chi_i(1,2,3,4). \tag{10}$$

The spin functions $\chi_i(1,2,3,4)$ in the above expression are as follows :

Singlet state functions :

$$\chi_1=\alpha(1)\beta(2)\alpha(3)\beta(4),$$
$$\chi_2=2^{-1/2}[\alpha(1)\beta(2)\alpha(3)\beta(4)-\alpha(1)\beta(2)\beta(3)\alpha(4)],$$
$$\chi_3=2^{-1}[\alpha(1)\beta(2)\alpha(3)\beta(4)-\beta(1)\alpha(2)\alpha(3)\beta(4)-\alpha(1)\beta(2)\beta(3)\alpha(4)+\beta(1)\alpha(2)\beta(3)\alpha(4)],$$
$$\chi_4=2^{-1}[\alpha(1)\alpha(2)\beta(3)\beta(4)-\beta(1)\alpha(2)\alpha(3)\beta(4)-\alpha(1)\beta(2)\beta(3)\alpha(4)+\beta(1)\beta(2)\alpha(3)\alpha(4)]. \tag{11}$$

Triplet state functions :

$$\chi_5=\alpha(1)\beta(2)\alpha(3)\alpha(4),$$
$$\chi_6=2^{-1/2}[\alpha(1)\beta(2)\alpha(3)\alpha(4)-\beta(1)\alpha(2)\alpha(3)\alpha(4)],$$
$$\chi_7=2^{-1/2}[\alpha(1)\alpha(2)\alpha(3)\beta(4)-\alpha(1)\alpha(2)\beta(3)\alpha(4)],$$
$$\chi_8=2^{-1}[\alpha(1)\alpha(2)\alpha(3)\beta(4)+\alpha(1)\alpha(2)\beta(3)\alpha(4)-\alpha(1)\beta(2)\alpha(3)\alpha(4)-\beta(1)\alpha(2)\alpha(3)\alpha(4)]. \tag{11a}$$

Quintet state function :

$$\chi_9 = \alpha(1)\alpha(2)\alpha(3)\alpha(4). \tag{11b}$$

Using these ASMO functions X_ν, we can compute the energy levels in the absence of CI, i.e., the levels according to the " single configuration approximation " by the expression :

$$E(X_\nu) = \int X_\nu^* \boldsymbol{H} X_\nu d\tau, \tag{12}$$

which can be expressed in terms of c_u, c_g (cf. Eq. (6)), S (Eq. (5)) and the molecular integrals, A, C, D, L listed in Table 2. Thus the numerical evaluation of these energies $E(X_\nu)$ is straightforward, the results being given in the third column of Table 1 and

Table 1. MO Functions for Various Configurations

Symmetry	Function X_ν	Energy, $E(X_\nu)$
$^1\Sigma_g^+$;	$A_1 = (u_+u_+u_-u_-; \chi_1)$	2.38 eV
	$A_2 = (u_+u_-g_+g_-; \chi_3)$	18.62
	$A_3 = (u_+u_-g_+g_-; \chi_4)$	25.71
	$A_4 = 2^{-1/2}[(u_+u_+g_-g_-; \chi_1) + (u_-u_-g_+g_+; \chi_1)]$	19.02
	$A_5 = (g_+g_+g_-g_-; \chi_1)$	36.17
$^1\Sigma_g^-$;	$B_1 = 2^{-1/2}[(u_+u_+g_-g_-; \chi_1) - (u_-u_-g_+g_+; \chi_1)]$	19.02
$^1\Sigma_u^+$;	$C_1 = 2^{-1/2}[(u_+u_+u_-g_-; \chi_2) + (u_-u_-u_+g_+; \chi_2)]$	19.95
	$C_2 = 2^{-1/2}[(g_+g_+g_-u_-; \chi_2) + (g_-g_-g_+u_+; \chi_2)]$	36.85
$^1\Sigma_u^-$;	$D_1 = 2^{-1/2}[(u_+u_+u_-g_-; \chi_2) - (u_-u_-u_+g_+; \chi_2)]$	8.01
	$D_2 = 2^{-1/2}[(g_+g_+g_-u_-; \chi_2) - (g_-g_-g_+u_+; \chi_2)]$	24.91
$^1\Delta_g$;	$E_1 = (u_+u_+g_+g_-; \chi_2)$, $E_1^* = (u_-u_-g_-g_+; \chi_2)$	17.48
	$E_2 = (g_+g_+u_+u_-; \chi_2)$, $E_2^* = (g_-g_-u_-u_+; \chi_2)$	17.48
$^1\Delta_u$;	$F_1 = (u_+u_+u_-g_+; \chi_2)$, $F_1^* = (u_-u_-u_+g_-; \chi_2)$	8.62
	$F_2 = (g_+g_+g_-u_+; \chi_2)$, $F_2^* = (g_-g_-g_+u_-; \chi_2)$	25.52
$^1\Gamma_g$;	$G_1 = (u_+u_+g_+g_+; \chi_1)$, $G_1^* = (u_-u_-g_-g_-; \chi_1)$	13.66
$^3\Sigma_g^+$;	$H_1 = (u_+u_-g_+g_-; \chi_8)$	18.38
$^3\Sigma_g^-$;	$I_1 = (u_+u_-g_+g_-; \chi_6)$	16.34
	$I_2 = (u_+u_-g_+g_-; \chi_7)$	16.34
$^3\Sigma_u^+$;	$J_1 = 2^{-1/2}[(u_+u_+u_-g_-; \chi_5) + (u_-u_-u_+g_+; \chi_5)]$	5.93
	$J_2 = 2^{-1/2}[(g_+g_+g_-u_-; \chi_5) + (g_-g_-g_+u_+; \chi_5)]$	22.82
$^3\Sigma_u^-$;	$K_1 = 2^{-1/2}[(u_+u_+u_-g_-; \chi_5) - (u_-u_-u_+g_+; \chi_5)]$	8.01
	$K_2 = 2^{-1/2}[(g_+g_+g_-u_-; \chi_5) - (g_-g_-g_+u_+; \chi_5)]$	24.91
$^3\Delta_g$;	$L_1 = (u_+u_+g_+g_-; \chi_5)$, $L_1^* = (u_-u_-g_-g_+, \chi_5)$	15.19
	$L_2 = (g_+g_+u_+u_-; \chi_5)$, $L_2^* = (g_-g_-u_-u_+; \chi_5)$	15.19
$^3\Delta_u$;	$M_1 = (u_+u_+u_-g_+; \chi_5)$, $M_1^* = (u_-u_-u_+g_-; \chi_5)$	6.97
	$M_2 = (g_+g_+g_-u_+; \chi_5)$, $M_2^* = (g_-g_-g_+u_-; \chi_5)$	23.86
$^5\Sigma_g^+$;	$N_1 = (u_+u_-g_+g_-; \chi_9)$	9.72

Table 2. Two-Electron Integrals*

In this table the abbreviation

$$(ab\,;cd)=\iint a(1)^*b(1)\,(1/r_{12})c(2)^*d(2)\,d\tau_1 d\tau_2$$

is used.

$A=(a_+a_+\,;\ a_+a_+)=(a_+a_+\,;\ a_-a_-)=16.017$ eV

$A'=(a_+a_-\,;a_-a_+)=1.825$ eV

$C=(a_+b_+\,;\ a_+b_+)=(a_+b_+\,;\ a_-b_-)=(a_+b_+\,;\ b_+a_+)=(a_+b_+\,;\ b_-a_-)=1.659$ eV

$C'=(a_+b_-\,;\ a_-b_+)=(a_+b_-\,;\ b_-a_+)=0.1844$ eV

$D=(a_+a_+\,;\ b_+b_+)=(a_+a_+\,;\ b_-b_-)=9.863$ eV

$D'=(a_+a_-\,;\ b_-b_+)=0.3732$ eV

$L=(a_+a_+\,;\ b_+a_+)=(a_+a_+\,;\ b_-a_-)=4.512$ eV

$L'=(a_+a_-\,;\ b_-a_+)=0.4004$ eV

illustrated in Fig. 2**. Here and hereafter, the zero of energy is shifted to $4E_{2p}-87.17$ eV, which is the position of the ${}^1\Sigma_g^+$ ground state energy level according to our calculation by the MO method with CI or the HL method with IHR (*vide infra*).

Let us now consider the effects of CI. For the ${}^1\Sigma_g^+$ state we have five ASMO functions $A_p\,(p=1,\cdots,5)$ (cf. Table 1), from which we construct the secular equation

$$\det(H_{pq}-E\Delta_{pq})=0,\quad (p,\,q=1,\cdots,5), \tag{13}$$

in which the matrix elements are given by

$$H_{pq}=\int A_p^*\,\boldsymbol{H}A_q d\tau,\quad \Delta_{pq}=\int A_p^*\,A_q\,d\tau. \tag{14}$$

The new ${}^1\Sigma_g^+$ state levels resulting from the inclusion of CI are given as the roots of the above secular equation, and the new wave functions associated with these levels are expressed as linear combinations of $A_1,\cdots A_5$, whose coefficients are also derived from Eq. (13). The effects of CI on the states of other symmetries and multiplicities are calculated similarly. Of course, the ${}^1\Sigma_g^-$, ${}^1\Gamma_g$, ${}^3\Sigma_g^+$ and ${}^3\Sigma_g^+$ states are not subject to CI (cf. Table 1). These results are summarized in Table 3 and Fig. 2, in which the levels corresponding to the roots other than the lowest ones of the secular equations are not included, because the energies of these levels are too high (>10 eV) for our approximation to be valid[7].*** In Table 3, the second, third and fourth columns give the new levels, the level depressions due to CI and the new wave functions respectively. These results will be discussed in Section 5.

* For the method of evaluation of these integrals, see Appendix. Since the functions a_- and b_- are the complex conjugates of a_+ and b_+, we can easily see that

$$(a_+a_+\,;\ a_+a_+)=(a_-a_-\,;\ a_-a_-),\quad (a_+b_+\,;\ a_+b_+)=(a_-b_-\,;\ a_-b_-)$$

and so on.

** In Fig. 2 the levels higher than 20 eV are not included.

*** Some levels in Table 3 or Fig. 2, although they correspond to the lowest roots of the secular equations, are also too high, and thus we cannot put much trust in the calculated positions of these levels.

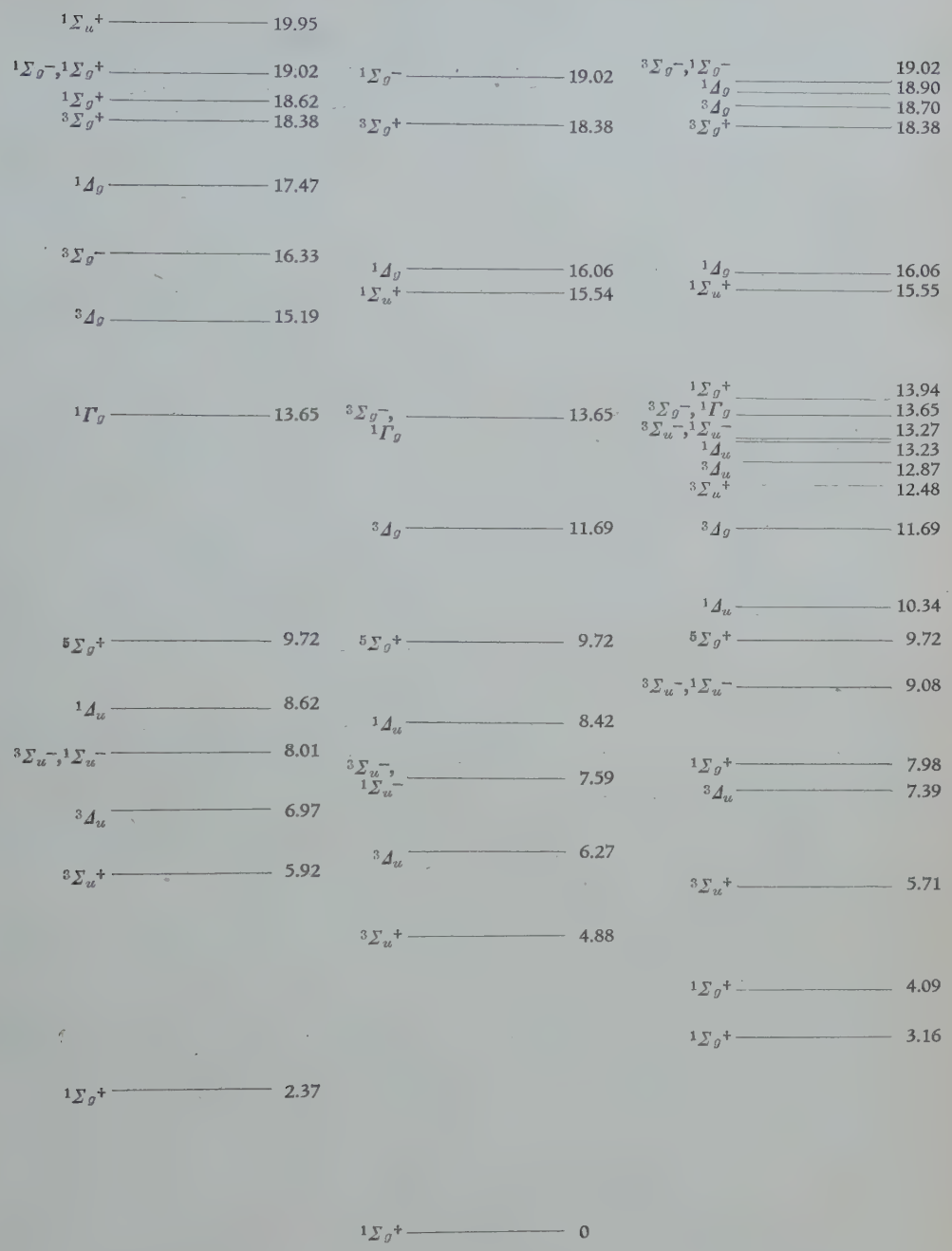
$^1\Sigma_u^+$ 19.95
$^1\Sigma_g^-, ^1\Sigma_g^+$ 19.02
$^1\Sigma_g^+$ 18.62
$^3\Sigma_g^+$ 18.38
$^1\Delta_g$ 17.47
$^3\Sigma_g^-$ 16.33
$^3\Delta_g$ 15.19
$^1\Gamma_g$ 13.65
$^5\Sigma_g^+$ 9.72
$^1\Delta_u$ 8.62
$^3\Sigma_u^-, ^1\Sigma_u^-$ 8.01
$^3\Delta_u$ 6.97
$^3\Sigma_u^+$ 5.92
$^1\Sigma_g^+$ 2.37
$^1\Sigma_g^-$ 19.02
$^3\Sigma_g^+$ 18.38
$^1\Delta_g$ 16.06
$^1\Sigma_u^+$ 15.54
$^3\Sigma_g^-, ^1\Gamma_g$ 13.65
$^3\Delta_g$ 11.69
$^5\Sigma_g^+$ 9.72
$^1\Delta_u$ 8.42
$^3\Sigma_u^-, ^1\Sigma_u^-$ 7.59
$^3\Delta_u$ 6.27
$^3\Sigma_u^+$ 4.88
$^1\Sigma_g^+$ 0
$^3\Sigma_g^-, ^1\Sigma_g^-$ 19.02
$^1\Delta_g$ 18.90
$^3\Delta_g$ 18.70
$^3\Sigma_g^+$ 18.38
$^1\Delta_g$ 16.06
$^1\Sigma_u^+$ 15.55
$^1\Sigma_g^+$ 13.94
$^3\Sigma_g^-, ^1\Gamma_g$ 13.65
$^3\Sigma_u^-, ^1\Sigma_u^-$ 13.27
$^1\Delta_u$ 13.23
$^3\Delta_u$ 12.87
$^3\Sigma_u^+$ 12.48
$^3\Delta_g$ 11.69
$^1\Delta_u$ 10.34
$^5\Sigma_g^+$ 9.72
$^3\Sigma_u^-, ^1\Sigma_u^-$ 9.08
$^1\Sigma_g^+$ 7.98
$^3\Delta_u$ 7.39
$^3\Sigma_u^+$ 5.71
$^1\Sigma_g^+$ 4.09
$^1\Sigma_g^+$ 3.16
Energies of Configurations (MO)
Final Results by MO with CI or HL with IHR
Energies of Structures (HL)

Fig. 2

Table 3. Levels and Wave Functions after Inclusion of CI or IHR

Symmetry	Energy	Depression by CI	Wave Function in Terms of MO Functions	Wave Function in Terms of HL Functions
$^1\Sigma_g^+$;	eV 0.00	eV 2.38	$\begin{cases}0.954A_1+0.139A_2+0\ 106A_3\\ -0.204A_4+0.063A_5\end{cases}$	$\begin{cases}-0.650A_a+0.149A_b+0.264A_c\\ +0.350A_d-0.020A_e\end{cases}$
$^1\Sigma_g^-$;	19.02	None	B_1	B_a
$^1\Sigma_u^+$;	15.54	4.41	$0.910C_1-0.414C_2$	$0.983C_a+0.027C_b$
$^1\Sigma_u^-$;	7.59	0.42	$0.988D_1+0.153D_2$	$0.725D_a\pm0.371D_b$
$^1\Delta_g$;	16.06	1.42	$2^{-1/2}(E_1+E_2)$ or $2^{-1/2}(E_1^*+E_2^*)$	E_a or E_a^*
$^1\Delta_u$;	8.42	0.20	$\begin{cases}0.994F_1+0.107F_2\\ \text{or } 0.994F_1^*+0.107F_2^*\end{cases}$	$\begin{cases}0.676F_a+0.427F_b\\ \text{or } 0.676F_a^*+0.427F_b^*\end{cases}$
$^1\Gamma_g$;	13.66	None	G_1 or G_1^*	G_a or G_a^*
$^3\Sigma_g^+$;	18.38	None	H_1	H_a
$^3\Sigma_g^-$;	13.66	2.68	$2^{-1/2}(I_1+I_2)$	I_a
$^3\Sigma_u^+$;	4.88	1.05	$0.972J_1+0.235J_2$	$0.811J_a-0.267J_b$
$^3\Sigma_u^-$;	7.59	0.42	$0.988K_1+0.153K_2$	$0.752K_a-0.371K_b$
$^3\Delta_g$;	11.69	3.51	$2^{-1/2}(L_1+L_2)$ or $2^{-1/2}(L_1^*+L_2^*)$	L_a or L_a^*
$^3\Delta_u$;	6.27	0.70	$\begin{cases}0.981M_1+0.195M_2\\ \text{or } 0.981M_1^*+0.195M_2^*\end{cases}$	$\begin{cases}0.769M_a-0.319M_b\\ \text{or } 0.769M_a^*-0.319M_b^*\end{cases}$
$^5\Sigma_g^+$;	9.72	None	N_1	N_a

§ 4. Calculation by HL method

Our problem of the four interacting $2p\pi$-electrons in the acetylene molecule can also be treated by the HL theory, with the use of atomic orbitals instead of molecular ones. In terms of the complex $2p\pi$ orbital functions $a_\pm$ and $b_\pm$, the ground state structure of this molecule will be $a_+\cdot b_+)\ a_-\cdot b_-)$, and further there will be excited homopolar structures $a_+\cdot a_-)b_+\cdot b_-)$, $a_+)^2b_-)^2$ etc.,* and ionic structures $a_+)^2a_-\cdot b_-)$, $a_+)^2a_-)^2$ etc. Taking all the excited homopolar and ionic structures within the frame of $(2p\pi)^4$, we obtain the HL type molecular wave functions X_i of various symmetries and multiplicities as shown in Table 4, where the same abbreviation as used in Table 1 (cf. Eq. (10)) is used. The appearance of the additional normalization factors $(1+S^2)^{-1}$ *etc.* in these functions is due to the non-orthogonality** between the atomic orbitals $a_\pm$ and $b_\pm$. The (electronic) " structures " corresponding to these HL functions are given in the third column of Table 4. The energies of the functions X_i, i.e., the energies of the " structures " are given by the integral

$$E(X_i)=\int X_i^*\boldsymbol{H}X_i d\tau,$$

* Here we use Mulliken's symbolism (J. Chem. Phys. **19** (1951), 900). Thus in the symbols $a_+\cdot b_+)$ $a_-\cdot b_-)$, $a_+)^2b_-)^2$ etc., the dots connect orbitals for electrons forming a pair bond, and $a_+)^2$ indicates two electrons forming a lone-pair in the orbital a_+, and so on.

** This non-orthogonality makes the computation by the HL method more cumbersome than that by the MO method.

Table 4. HL Functions for Various Structures*

Symmetry	Function X_i	Structure	Energy
$^1\Sigma_g^+$;	$A_a=(1+S^2)^{-1}(a_+a_-b_+b_-;\ \chi_4)$	$a_+\cdot a_+)\ a_-\cdot b_-)$	3.16 eV
	$A_b=(1-S^2+S^4)^{-1/2}(a_+a_-b_+b_-;\ \chi_3)$	$a_+\cdot a_-)\ b_+\cdot b_-)$	13.94
	$A_c=(2+2S^4)^{-1/2}[(a_+a_+b_-b_-;\ \chi_1)+(a_-a_-b_+b_+;\ \chi_1)]$	$a_+)^2b_-)^2$	7.98
	$A_d=2^{-1}(1+6S^2+S^4)^{-1/2}[(\mathrm{I})+(\mathrm{II})+(\mathrm{III})+(\mathrm{IV})]$	$a_+)^2a_-\cdot b_-)$	4.09
	$A_e=(2+2S^4)^{-1/2}[(a_+a_+a_-a_-;\ \chi_1)+(b_+b_+b_-b_-;\ \chi_1)]$	$a_+)^2a_-)^2$	29.04
$^1\Sigma_g^-$;	$B_a=2^{-1}(1-S^2)^{-1}[(\mathrm{I})+(\mathrm{II})-(\mathrm{III})-(\mathrm{IV})]$	$a_+)^2a_-\cdot b_-)$	19.02
$^1\Sigma_u^+$;	$C_a=2^{-1}(1-S^4)^{-1/2}[(\mathrm{I})-(\mathrm{II})+(\mathrm{III})-(\mathrm{IV})]$	$a_+)^2a_-\cdot b_-)$	15.55
	$C_b=(2-2S^4)^{-1/2}[(a_+a_+a_-a_-;\ \chi_1)-(b_+b_+b_-b_-;\ \chi_1)]$	$a_+)^2a_-)^2$	30.70
$^1\Sigma_u^-$;	$D_a=(2-2S^4)^{-1/2}[(a_+a_+b_-b_-;\ \chi_1)-(a_-a_-b_+b_+;\ \chi_1)]$	$a_+)^2b_-)^2$	9.08
	$D_b=2^{-1}(1-S^4)^{-1/2}[(\mathrm{I})-(\mathrm{II})-(\mathrm{III})+(\mathrm{IV})]$	$a_+)^2a_-\cdot b_-)$	13.27
$^1\Delta_g$;	$E_a=2^{-1/2}(1-S^2)^{-1}[(a_+a_+b_+b_-;\ \chi_2)+(b_+b_+a_+a_-;\ \chi_2)]$	$a_+)^2b_+\cdot b_-)$	16.06
	$E_a{}^*=2^{-1/2}(1-S^2)^{-1}[(a_-a_-b_-b_+;\ \chi_2)+(b_-b_-a_-a_+;\ \chi_2)]$	$a_+)^2b_+\cdot b_-)$	
	$E_b=2^{-1/2}(1-S^2)^{-1}[(a_+a_+a_-b_+;\ \chi_2)+(b_+b_+b_-a_+;\ \chi_2)]$	$a_+)^2a_-\cdot b_+)$	18.90
	$E_b{}^*=2^{-1/2}(1-S^2)^{-1}[(a_-a_-a_+b_-;\ \chi_2)+(b_-b_-b_+a_-;\ \chi_2)]$	$a_+)^2a_-\cdot b_+)$	
$^1\Delta_u$;	$F_a=2^{-1/2}(1-S^4)^{-1/2}[(a_+a_+b_+b_-;\ \chi_2)-(b_+b_+a_+a_-;\ \chi_2)]$	$a_+)^2b_+\cdot b_-)$	10.34
	$F_a{}^*=2^{-1/2}(1-S^4)^{-1/2}[(a_-a_-b_-b_+;\ \chi_2)-(b_-b_-a_-a_+;\ \chi_2)]$	$a_+)^2b_+\cdot b_-)$	
	$F_b=2^{-1/2}(1-S^4)^{-1/2}[(a_+a_+a_-b_+;\ \chi_2)-(b_+b_+b_-a_+;\ \chi_2)]$	$a_+)^2a_-\cdot b_+)$	13.23
	$F_b{}^*=2^{-1/2}(1-S^4)^{-1/2}[(a_-a_-a_+b_-;\ \chi_2)-(b_-b_-b_+a_-;\ \chi_2)]$	$a_+)^2a_-\cdot b_+)$	
$^1\Gamma_g$;	$G_a=(1-S^2)^{-1}(a_+a_+b_+b_+;\ \chi_1)$	$a_+)^2b_+)^2$	13.66
	$G_a{}^*=(1-S^2)^{-1}(a_-a_-b_-b_-;\ \chi_1)$	$a_+)^2b_+)^2$	
$^3\Sigma_g^+$;	$H_a=2^{-1}(1-S^2)^{-1}[(\mathrm{i})+(\mathrm{ii})+(\mathrm{iii})+(\mathrm{iv})]$	$a_+)^2a_-)b_-)$	18.38
$^3\Sigma_g^-$;	$I_a=2^{-1/2}(1-S^2)^{-1}[(a_+a_-b_+b_-;\ \chi_6)+(a_+a_-b_+b_-;\ \chi_7)]$	$a_+\cdot a_-)b_+)b_-)$	13.66
	$I_b=2^{-1}(1-S^2)^{-1}[(\mathrm{i})+(\mathrm{ii})-(\mathrm{iii})-(\mathrm{iv})]$	$a_+)^2a_-)b_-)$	19.02
$^3\Sigma_u^+$;	$J_a=(1-S^4)^{-1/2}(a_+a_-b_+b_-;\ \chi_8)$	$a_+\cdot b_+)a_-)b_-)$	5.71
	$J_b=2^{-1}(1-S^4)^{-1/2}[(\mathrm{i})-(\mathrm{ii})+(\mathrm{iii})-(\mathrm{iv})]$	$a_+)^2a_-)b_-)$	12.48
$^3\Sigma_u^-$;	$K_a=2^{-1/2}(1-S^4)^{-1/2}[(a_+a_-b_+b_-;\ \chi_6)-(a_+a_-b_+b_-;\ \chi_7)]$	$a_+\cdot a_-)b_+)b_-)$	9.08
	$K_b=2^{-1}(1-S^4)^{-1/2}[(\mathrm{i})-(\mathrm{ii})-(\mathrm{iii})+(\mathrm{iv})]$	$a_+)^2a_-)b_-)$	13.27
$^3\Delta_g$;	$L_a=2^{-1/2}(1-S^2)^{-1}[(a_+a_+b_+b_-;\ \chi_5)+(b_+b_+a_+a_-;\ \chi_5)]$	$a_+)^2b_+)b_-)$	11.69
	$L_a{}^*=2^{-1/2}(1-S^2)^{-1}[(a_-a_-b_-b_+;\ \chi_5)+(b_-b_-a_-a_+;\ \chi_5)]$	$a_+)^2b_+)b_-)$	
	$L_b=2^{-1/2}(1-S^2)^{-1}[(a_+a_+a_-b_+;\ \chi_5)+(b_+b_+b_-a_+;\ \chi_5)]$	$a_+)^2a_-)b_+)$	18.70
	$L_b{}^*=2^{-1/2}(1-S^2)^{-1}[(a_-a_-a_+b_-;\ \chi_5)+(b_-b_-b_+a_-;\ \chi_5)]$	$a_+)^2a_-)b_+)$	
$^3\Delta_u$;	$M_a=2^{-1/2}(1-S^4)^{-1/2}[(a_+a_+b_+b_-;\ \chi_5)-(b_+b_+a_+a_-;\ \chi_5)]$	$a_+)^2b_+)b_-)$	7.39
	$M_a{}^*=2^{-1/2}(1-S^4)^{-1/2}[(a_-a_-b_-b_+;\ \chi_5)-(b_-b_-a_-a_+;\ \chi_5)]$	$a_+)^2b_+)b_-)$	
	$M_b=2^{-1/2}(1-S^4)^{-1/2}[(a_+a_+a_-b_+;\ \chi_5)-(b_+b_+b_-a_+;\ \chi_5)]$	$a_+)^2a_-)b_+)$	12.87
	$M_b{}^*=2^{-1/2}(1-S^4)^{-1/2}[(a_-a_-a_+b_-;\ \chi_5)-(b_-b_-b_+a_-;\ \chi_5)]$	$a_+)^2a_-)b_+)$	
$^5\Sigma_g^+$;	$N_a=(1-S^2)^{-1}(a_+a_-b_+b_-;\ \chi_9)$	$a_+)\ a_-)b_+)b_-)$	9.72

* In order to make this table compact, we have used the following abbreviations in the second column:

(I) $=(a_+a_+a_-b_-;\ \chi_2)$, (II) $=(b_+b_+b_-a_-;\ \chi_2)$, (III) $=(a_-a_-a_+b_+;\ \chi_2)$, (IV) $=(b_-b_-b_+a_+;\ \chi_2)$,

(i) $=(a_+a_+a_-b_-;\ \chi_5)$, (ii) $=(b_+b_+b_-a_-;\ \chi_5)$, (iii) $=(a_-a_-a_+b_+;\ \chi_5)$, (iv) $=(b_-b_-b_+a_+;\ \chi_5)$.

which can be expressed in terms of the molecular integrals S, I, F, A, D, C and L (see Eqs. (5), (7) and Table 2). The numerical values of $E(X_i)$ are given in the fourth column of Table 4. In Table 4, of course, we have the same number of functions for each symmetry and multiplicity as in the MO case. In fact, for each symmetry and multiplicity, the HL functions are expressed as linear combinations of the MO functions, and these linear relations are easily found to be as follows :*

$$
{}^1\Sigma_g^+;\quad \begin{pmatrix} (1+S^2)A_a \\ (1-S^2+S^4)^{1/2}A_b \\ (1+S^4)^{1/2}A_c \\ (1+6S^2+S^4)^{1/2}A_d \\ (1+S^4)^{1/2}A_e \end{pmatrix} = \frac{1}{4}\begin{pmatrix} -2 & 0 & 0 & \sqrt{8} & -2 \\ -1 & 4 & -2 & \sqrt{2} & -1 \\ \sqrt{2} & 0 & \sqrt{8} & 2 & \sqrt{2} \\ \sqrt{8} & 0 & 0 & 0 & -\sqrt{8} \\ \sqrt{2} & 0 & -\sqrt{8} & 2 & \sqrt{2} \end{pmatrix} \begin{pmatrix} N_u^2 A_1 \\ N_u N_g A_2 \\ N_u N_g A_3 \\ N_u N_g A_4 \\ N_g^2 A_5 \end{pmatrix},
$$

$$
{}^1\Sigma_g^-;\quad B_a = B_1,
$$

$$
{}^1\Sigma_u^+;\quad \begin{pmatrix} TC_a \\ TC_b \end{pmatrix} = \sqrt{\tfrac{1}{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} NC_1 \\ N'C_1 \end{pmatrix}, \qquad {}^1\Sigma_u^-;\quad \begin{pmatrix} TD_a \\ TD_b \end{pmatrix} = \sqrt{\tfrac{1}{2}}\begin{pmatrix} -1 & -1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} ND_1 \\ N'D_2 \end{pmatrix},
$$

$$
{}^1\Delta_g;\quad \begin{pmatrix} E_a \\ E_b \end{pmatrix} = \sqrt{\tfrac{1}{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} E_1 \\ E_2 \end{pmatrix}, \qquad {}^1\Delta_u;\quad \begin{pmatrix} TF_a \\ TF_b \end{pmatrix} = \sqrt{\tfrac{1}{2}}\begin{pmatrix} -1 & -1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} NF_1 \\ N'F_2 \end{pmatrix},
$$

$$
{}^1\Gamma_g;\quad G_a = G_1, \qquad {}^3\Sigma_g^+;\quad H_a = H_1,
$$

$$
{}^3\Sigma_g^-;\quad \begin{pmatrix} I_a \\ I_b \end{pmatrix} = \sqrt{\tfrac{1}{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} I_1 \\ I_2 \end{pmatrix}, \qquad {}^3\Sigma_u^+;\quad \begin{pmatrix} TJ_a \\ TJ_b \end{pmatrix} = \sqrt{\tfrac{1}{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} NJ_1 \\ N'J_2 \end{pmatrix},
$$

$$
{}^3\Sigma_u^-;\quad \begin{pmatrix} TK_a \\ TK_b \end{pmatrix} = \sqrt{\tfrac{1}{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} NK_1 \\ N'K_2 \end{pmatrix}, \qquad {}^3\Delta_g;\quad \begin{pmatrix} L_a \\ L_b \end{pmatrix} = \sqrt{\tfrac{1}{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} L_1 \\ L_2 \end{pmatrix},
$$

$$
{}^3\Delta_u;\quad \begin{pmatrix} TM_a \\ TM_b \end{pmatrix} = \sqrt{\tfrac{1}{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} NM_1 \\ N'M_2 \end{pmatrix}, \qquad {}^5\Sigma_g^+;\quad N_a = N_1. \tag{15}
$$

On finding these interrelations between the wave functions of MO and HL types, it would be superfluous to calculate the interaction among the different HL structures, since all the matrix elements H_{pq} or Δ_{pq} (Eq. (14)) in the HL case can be easily derived from those in the MO case by the use of the above interrelations (15), and since the final results to be arrived at should coincide with the results of Section 3. Nevertheless we carried out these calculations and solved the secular equations independently of those obtained in Section 3. The agreement of these results with those of Section 3 served as a useful check for our numerical computation. In the last column of Table 3 the eigenfunctions corresponding to the lowest roots of the secular equations are given in terms of the HL wave functions. Of course these eigenfunctions are identical with the

* For brevity of the expressions, the following abbreviations are used here:

$$
T=(1-S^4)^{1/2}, \qquad N=(N_u^3 N_g)^{1/2}, \qquad N'=(N_u N_g^3)^{1/2}.
$$

corresponding ones obtained by the MO method with CI.

§ 5. Discussion

The results of our calculation show that the effect of CI in the MO case or of IHR in the HL case on the energy levels is fairly large, amounting to several electron volts. Similar results have been obtained in the case of hydrocarbons with conjugate double bonds by Craig and others[4)-7)].

Now let us consider the MO case. From the inspection of Fig. 2, which illustrates our results, we must conclude that no simple and general relation seems to exist between the amount of level depression and the spatial symmetry as well as the spin multiplicity of the state, thus it is difficult to find out the "criteria for the selection of configurations" mentioned in Introduction. This situation has already been pointed out and called "melancholic" by Coulson *et al.*[7)] The largest shift 4.41 eV is found for the $^1\sum_u^+$ state. In the case of $^3\Delta_g$, $^1\Delta_g$ or $^3\sum_g^-$, two energy levels by the single configuration approximation accidentally degenerate, which is responsible for the large shift by CI. The shift of $^3\Delta_g$ level is much larger than that of the $^1\Delta_g$ level, which is contrary to Coulson's statement[7)] that the effect of CI in a triplet state is less than it would be in a singlet state if otherwise comparable.

By using the relation (15) we can express the MO wave function A_1 for the lowest $^1\sum_g^+$ configuration in terms of the HL functions* as follows:

$$A_1 = -0.308A_a + 0.195A_c + 0.513A_d + 0.195A_e\,, \tag{16}$$

which contains a considerable amount of the ionic functions A_d and A_e (cf. Table 4). This is compared with the "true" wave function for the $^1\sum_g^+$ ground state (cf. Table 3),

$$-0.650A_a + 0.149A_b + 0.264A_c + 0.350A_d - 0.020A_e\,, \tag{17}$$

which shows how the inclusion of CI has reduced the superfluity of ionic terms[8)].

Eq. (17) shows also that the "true" wave function for the $^1\sum_g^+$ ground state involves rather large contributions from the homopolar lone-pair structure A_c and the singly ionic structure A_d. Thus we might expect that the fairly good approximation for $^1\sum_g^+$ ground state can be obtained by considering the resonance only between A_a and A_d, or only between A_a and A_c. This is confirmed by computations, the results of which are illustrated in Fig. 3**.

Another approximation to the $^1\sum_g^+$ ground state function can be made by the use of the HL function

---

* While the MO functions A_1, A_2,……, etc. are mutually orthogonal except that $\Delta_{23} = \int A^*_2 A_3 d\tau = \frac{1}{2}$, the HL functions A_a, A_b,……, etc. lack this orthogonality. For instance,

$\Delta_{ab} = 0.5944$, $\Delta_{ac} = -0.3073$, $\Delta_{ad} = -0\,7490$, $\Delta_{ae} = -0.3073$,
$\Delta_{bc} = -0.1826$, $\Delta_{bd} = -0.4452$, $\Delta_{be} = -0.1826$, $\Delta_{cd} = 0.5903$,
$\Delta_{ce} = 0.2421$, $\Delta_{de} = 0.5903$.

** In Fig. 3 the level obtained by considering the resonance between A_a and A_c is labelled by $(A_a - A_c)$, and so on.

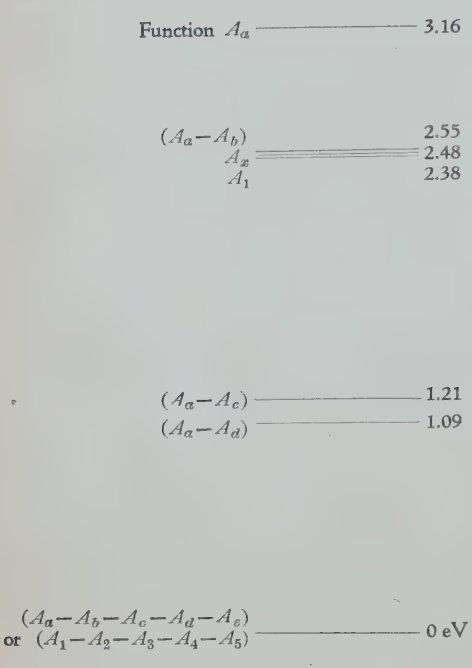

Fig. 3

$$A_x=(1+2S^2+S^4)^{-1/2}(a_x a_y b_x b_y\,;\,\chi_4), \tag{18}$$

where the abbreviation (10) is used, and a_x, a_y, b_x, b_y are the real $2p\pi$ atomic orbital functions:

$$\begin{aligned} a_x&=2^{-1/2}(a_+ + a_-),\\ a_y&=2^{-1/2}\,i^{-1}(a_+ - a_-),\\ b_x&=2^{-1/2}(b_+ + b_-),\\ b_y&=2^{-1/2}\,i^{-1}(b_+ - b_-). \end{aligned} \tag{19}$$

This wave function representing the electronic structure $a_x\cdot b_x)\ \ a_y\cdot b_y)$, has often been used for the description of the electronic structure of a triple bond.[13] However, this function lacks the axial symmetry $({}^1\Sigma_g^+)$ of the ground state, because these real $2p\pi$ orbitals possess a marked directional property around the molecular axis. In fact this function can be expressed in terms of the HL functions given in Table 4 as follows:

$$A_x=-1.000A_a+0.421A_b+0.317A_c-0.195(G_a+G_a^*), \tag{20}$$

which includes the functions G_a and G_a^* of symmetry ${}^1\Gamma_g$. Nevertheless, on evaluating the integral $E(A_x)=\int A_x^*\,\boldsymbol{H}\,A_x\,d\tau$, we find that the energy of this function is fairly low:

$$E(A_x)=2.48\text{ eV}.$$

In terms of Eq. (20), we can attribute this fact to the strong interactions among the functions A_a, A_b and A_c (*vide supra*). Thus we see that this function A_x is preferable to A_a for the purpose of single structure approximation for the ${}^1\Sigma_g^+$ ground state.

The observations and analyses of the near ultra-violet spectra of acetylene have not yet been completely made so far as the authors know. Woo *et al.*[11] observed the spectrum extending from 2430 *A* down to the ultra-violet limit of their instrument, and considered the band to be due to a forbidden transition. On the other hand, our calculation shows that several excited levels lie in the neighborhood of 5 eV (cf. Table 3), the energy difference of 5 eV corresponding to a transition of 2500 A. From the symmetries of these levels, we see that the transitions from the ground state to these levels are forbidden.[12] However, because of the poverty of the experimental data, a satisfactory comparison of our calculated results with the experiments seems to be impossible for the present.

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Appendix

In this appendix the evaluation of the molecular integrals occurring in our calculation is explained. The numerical values of these integrals given here and in Table 2 are for $2\delta R=7.22$, where $2\delta=3.18$ is the screening constant (cf. Eq. (1)) and $R=2.27$ a.u. the internuclear distance.

A. The overlap integral S is easily evaluated using the formula given by Kotani *et al.*[17] or by Mulliken *et al.*[14] :

$$S=0.35057.$$

B. To evaluate the one-electron integrals I and F we proceed as follows. Using the definition (7) and the relation (8) of Section 3, we can write as

$$I=E_{2p}-A-2D-K, \quad F=SE_{2p}-3L-J.$$

In these expressions, A, D and L are the integrals defined in Table 2; K and J are Mayer and Sklar's Coulomb and exchange penetration integrals[3] respectively; *i.e.*

$$K=-\int a_+^*(q)\left[-(4/r_{bq})+\int (1/r_{jq})\rho(j)d\tau_j\right]a_+(q)d\tau_q=1.6959 \text{ eV},$$

$$J=-\int b_+^*(q)\left[-(4/r_{bq})+\int (1/r_{jq})\rho(j)d\tau_j\right]a_+(q)d\tau_q=3.1176 \text{ eV},$$

with $$\rho(j)=|b_-(j)|^2+|b_+(j)|^2+|b_{2s}(j)|^2+|b_{2p\sigma}(j)|^2.$$

The formulae for the evaluation of K and J are given in Parr and Crawford's paper.[16] It may, however, be more convenient to compute the latter integral J with the alternative formula*,

$$\begin{aligned}\delta^{-1}J=(\delta R/2)^5\big[&8(\delta R)^{-1}\{-A_2(B_2-B_0)+A_2(B_3-B_1)+A_1(B_2-B_0)-A_0(B_3-B_1)\}\\&+6\{-A_4(B_2-B_0)+A_2(B_4-B_0)-A_0(B_4-B_2)\}+2\delta R\{-A_5(B_2-B_0)\\&-A_4(B_3-B_1)+A_3(B_4-B_0)+A_2(B_5-B_1)-A_1(B_4-B_2)-A_0(B_5-B_3)\}\\&+\tfrac{1}{2}(\delta R)^2\{-A_6(B_2-B_0)-2A_5(B_3-B_1)+A_4(B_2-B_0)+2A_3(B_5-B_1)\\&+A_2(B_6-B_4)-2A_1(B_5-B_3)-A_0(B_6-B_4)\}\big],\end{aligned}$$

where

$$A_m=A_m(2\delta R)=\int_1^\infty \exp(-2\delta R\lambda)\lambda^m d\lambda,$$

and

$$B_m=B_m(\delta R)=\int_{-1}^1 \exp(-\delta R\lambda)\lambda^m d\lambda,$$

are the integrals defined by Zener.[15]**

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* This can be obtained by using elliptic coordinates.

** The extensive numerical tables of these integrals are given in ref. 17.

C. The integrals A and A' have been evaluated by Parr and Crawford[16]; C, C', D, D', L and L' are evaluated by the use of the formulae and numerical tables given by Kotani *et al.*[17]*

* Parr and Crawford, Mulliken *et al.*, and Kotani *et al.* have given the formulae and tables for the integrals over the real $2p\pi$ functions, while our integrals are those over the complex $2p'\pi$ functions. However, the derivation of the latter integrals from the former is a very simple matter.

References

1) S. Altmann, Proc. Roy. Soc. London **A210** (1952), 327;
C. A. Coulson, N. H. March and S. Altmann, Proc. Nat. Acad. Sci. **38** (1952), 372.
2) E. Hueckel, ZS. f. Physik **70** (1931), 204.
3) M. Goeppert-Mayer and A. L. Sklar, J. Chem. Phys. **6** (1938), 645.
4) D. P. Craig, Proc. Roy. Soc. London **A200** (1950), 474.
5) D. P. Craig, Proc. Roy. Soc. London **A202** (1950), 498.
6) C. A. Coulson and J. Jacobs, Proc. Roy. Soc. London **A206** (1951), 287.
7) C. A. Coulson, D. P. Craig and J. Jacobs, Proc. Roy. Soc. London **A206** (1951), 297.
8) J. H. Van Vleck and A Sherman, Rev. Mod. Phys. **7** (1935), 167.
9) C. Zener, Phys. Rev. **36** (1930), 51.
10) G. Herzberg, "*Infra-Red and Raman Spectra of Polyatomic Molecules*" (1945).
11) S. C. Woo, T.K. Liu, T.C. Chu and W. Chih, J. Chem. Phys. **6** (1938), 240.
12) H. Sponer and E. Teller, Rev. Mod. Phys. **13** (1941), 76.
13) Cf., for example, H.J. Kopineck, Z. f. Naturforsch. **7a** (1952), 314.
14) R. S. Mulliken, C. A. Rieke, D. Orloff and H. Orloff, J. Chem. Phys. **17** (1949), 1248.
15) C. Zener and V. Guillemin, Phys. Rev. **34** (1929), 999.
16) R. G. Parr and B. L. Crawford, J. Chem. Phys. **16** (1948), 1049.
17) M. Kotani, A. Amemiya and T. Simose, Proc. Phys. Math. Soc. Jap. **20** (1938) Extra No. 1.; K. Hijikata *et al.*, to be published.

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On Lagrangian Formalism

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The differences between Lagrangian and Hamiltonian formalisms are discussed through the concept of chronological ordering operators, thereby keeping close correspondence to Feynman's path integral.

Next a method to derive commutation relations without referring to Hamiltonian formalism is presented.

§ 1. Introduction

It has long been believed that some basic alterations of the field concept should be made in order to get rid of the divergence difficulties inherent in the present field theory. While the recent development of the renormalization theory has succeeded in consistently eliminating divergences from the theory in some special cases.

This is possible only when the theory is described in a manifestly covariant way, and for this purpose it is essentially important that Tomonaga–Schwinger's Hamiltonian formalism is equivalent to Feynman's Lagrangian formalism on which Dyson has developed his beautiful theory.

For practical purposes the two theories do not contradict each other, but the basic ideas from which they started are essentially dissimilar. We shall therefore investigate their differences in a unified manner through the concept of chronological ordering operators.

We shall first define the chronological ordering operators P and P^* (in § 2). Next we shall prove the equivalence of the two theories with the use of these operators (in § 3). Last, we shall present a method to derive commutation relations between field variables without referring to Hamiltonian formalism (in § 4).

§ 2. Chronological ordering operators

(I) *Dyson's chronological ordering operator P*

As is well known, the solution of the Schrödinger equation:

$$i\frac{\partial\psi}{\partial t}=H(t)\psi\,,\quad(\hbar=c=1) \tag{2·1}$$

can be written as[1]

$$\psi(t)=U(t,t_0)\psi(t_0),\quad U(t,t_0)=P_t\exp[-i\int_{t_0}^{t}H(t)dt]\,, \tag{2·2}$$

where P_t or simply P is an operator introduced by Dyson.

To define P, we introduce a one-parameter family of space-like surfaces filling the whole space-time, so that one and only one member $\sigma(x)$ of the family passes through any given point x.

If $Q_1(x_1), \cdots, Q_n(x_n)$ are any operators defined, respectively, at the points $x_1, \cdots, x_n$ of space-time, then

$$P[Q_1(x_1), \cdots, Q_n(x_n)] \tag{2·3}$$

will denote the product of these operators, taken in order, reading from right to left, in which the surfaces $\sigma(x_1), \cdots, \sigma(x_n)$ occur in time, which means that the one-parameter family of space-like surfaces is the defining system of the chronological ordering operator P.

We shall write the parameter as a suffix to the symbol P, if necessary, but shall omit it if time is the parameter.

It is noteworthy to refer that the expression (2·3) is family-independent if $Q_i(x_i)$ commutes with $Q_j(x_j)$ so long as x_i and x_j are outside each other's light cones. In other cases, the expression (2·3) is, indeed, family-dependent.

One of the characteristic features of the Hamiltonian formalism is that Hamiltonian is expressed as a function of the coordinate variable q and its canonically conjugate variable p:

$$H(t)=H[q(t), p(t)]. \tag{2·4}$$

Hence the meaning of $U(t, t_0)$ in the expression (2·2) is unique provided that the variables q and p in the Hamiltonian (2·4) are arranged definitely in order.

For different quantities Q and Q', we have from the definition of the operator P

$$P[Q(t)Q'(t')]=\begin{cases} Q(t)Q'(t'), & \text{for} \quad t>t' \\ Q'(t')Q(t), & \text{for} \quad t<t' \end{cases}$$

except for $t=t'$, when we suffer from the ambiguity how to define it if $Q(t)Q'(t') \neq Q'(t')Q(t)$. In the expression (2), however, we are fortunate to observe

$$Q_1=\cdots=Q_n=H.$$

We shall hereafter leave the definition of the operator P for $t=t'$ undefined, nevertheless it doesn't matter so long as the operator P appears in the integrand since the undefined domain of P is a point and consequently does not contribute to the integral.

With this attention, it is easily seen that the expression (2·2) indeed satisfies the equation (2·1):

$$\begin{aligned} i\frac{\partial}{\partial t}U(t, t_0) &= P[H(t), \exp\{-i\int_{t_0}^{t} H(t)dt\}] \\ &= P[H(t), \exp\{-i\int_{t_0}^{t-0} H(t)dt\}] \\ &= H(t)P[\exp\{-i\int_{t_0}^{t-0} H(t)dt\}]. \end{aligned} \tag{2·5}$$

It is because all quantities are regarded as "monopole quantities" that we can safely separate $H(t)$ from the operator P to the left. As for the definition of "monopole quantity" we shall give it in the later part of this section.

From the definition follows at once the fundamental properties of the operator P which are already utilized in the above proof (2·5).

(a) P is a linear operator, i. e.

$$P[cQ, c'Q', \cdots]=cc'\cdots P[Q, Q', \cdots],$$

where c, c' are c-numbers.

$$P[Q_1+Q_2, Q', \cdots]=P[Q_1, Q', \cdots]+P[Q_2, Q', \cdots].$$

(distributive law)

(b) P is a symmetric operator, i. e.

$$P[Q_1, Q_2, \cdots]=P[Q_{1'}, Q_{2'}, \cdots],$$

where $(1', 2', \cdots)$ is an arbitrary permutation of $(1, 2, \cdots)$.

Lastly, as a chronological ordering operator,

(c) If $t, t', \cdots > \tau, \tau', \cdots$,

$$P[Q(t)Q'(t')\cdots R(\tau)R'(\tau')\cdots]$$
$$=P[Q(t)Q'(t')\cdots]\cdot P[R(\tau)R'(\tau')\cdots].$$

(separable law)

(II) *Modified chronological operator* P^*

Next we shall glance at Feynman's Lagrangian formalism in connection with the definition of the operator P^*.

One of the characteristic features of the Lagrangian formalism is that Lagrangian is expressed as a function of the coordinate variable q and its time derivative $\dot{q}$ in place of canonically conjugate pair q and p:

$$L(t)=L[q(t), \dot{q}(t)]. \qquad (2\cdot6)$$

The transformation function in Feynman's theory is given in the q representation by[2)]

$$U(t, t_0)=\int\!\!\int_{-}^{-} \exp\left[i/\hbar \int_{t_0}^{t} L[q(t), \dot{q}(t)]\right] \mathfrak{D}(\text{path}). \qquad (2\cdot7)$$

Besides, as Feynman has pointed out, the multiplicative property of the transformation function:

$$U(t_2, t_0)=U(t_2, t_0)U(t_1, t_0) \qquad (2\cdot8)$$

follows only when the Lagrangian is a function of q and $\dot{q}$ and does not involve higher time derivatives, in other words, this condition requires that the Lagrangian cannot involve higher multipole quantities than "dipole quantity".

We shall call it as "separability condition".

In performing the path integral, we slice the time axis into N intervals of thickness ϵ, then we may approximate the integral over all paths by the multiple integral

$$U(t, t_0)=\int\cdots\int \exp\left\{\frac{i}{\hbar}\sum_{j=1}^{N-1} S(q_{j+1}, q_j)\right\}\frac{dq_2}{A}\cdots\frac{dq_{N-1}}{A}, \qquad (2\cdot 9)$$

where A is a suitable normalizing factor and

$$S(q_{i+1}, q_i)=\varepsilon L\left[q_i, \frac{\dot{q}_{i+1}-q_i}{\varepsilon}\right].$$

In carrying out the integration, we have replaced $\dot{q}(t)$ by

$$\dot{q}_i=(\lim_{\varepsilon\to 0})\frac{q(t_i+\varepsilon)-q(t_i)}{\varepsilon}=(\lim_{\varepsilon\to 0})\frac{q_{i+1}-q_i}{\varepsilon}, \qquad (2\cdot 10)$$

i. e., we have decomposed $\dot{q}(t)$ into q's of two adjacent times. The limiting procedure $(\lim_{\varepsilon\to 0})$ should be performed after the integration, which means that the procedure is to be performed after the time ordering. As is seen from above, $\dot{q}_i$ can be written as a linear combination of q's of two adjacent times $t_{i+1}=t_i+\varepsilon$ and t_i.

It is for this reason that we call $\dot{q}(t)$ as a "dipole quantity", and $q(t)$ as a "monopole quantity".[3)]

This is the most essential difference of the Lagrangian formalism from the Hamiltonian formalism, in which latter all quantities with a single parameter t are regarded as monopole quantities.

For instance, $p(t)=m\dot{q}(t)$ is regarded on the one hand as a monopole quantity in the Hamiltonian formalism with the chronological ordering operator I', while on the other hand it is a dipole quantity in the Lagrangian formalism.

This difference suggests us an idea that we ought to define another chronological ordering operator suited to Lagrangian formalism, corresponding to the operator I' in the Hamiltonian formalism.

First we must fix the independent (field) variables corresponding to the variable q in the path integral. It is also necessary for this purpose to determine which of the variables are monopole quantities.

The variables should be independent, otherwise the distinction between monopole and dipole quantities becomes ambiguous.

For instance, the four components ϕ_μ of the vector field are not independent since they are restricted from the field equation by

$$\frac{\partial\phi_\mu}{\partial x_\mu}=0,$$

and if we incorrectly chose ϕ_μ as independent field variables, $\dot{\phi}_0$ would be either a monopole quantity and at the same time a dipole quantity. In this case, we had better employ Stückelberg's formalism, and replace ϕ_μ by

$$\phi_\mu\to A_\mu+\frac{1}{\varkappa}\frac{\partial B}{\partial x_\mu},$$

then the restriction becomes a subsidiary condition on state vectors;

$$\left(\frac{\partial A_\mu}{\partial x_\mu}+\varkappa B\right)\Psi=0\,,$$

which is not derived from the field equation, and we can safely choose four A_μ and B as independent field variables.

We denote the independent field variables thus fixed by $q_i(i=1, 2, \cdots, f,\ f$: degrees of freedom), and define a new chronological ordering operator P^* as follows.[4]

The expression

$$P^*[Q_1(x_1), \cdots, Q_n(x_n)] \qquad (2\cdot11)$$

is obtained by decomposing the field quantities Q's into independent field variables q's, i. e., into linear combinations of monopole quantities, then arranging them in order defined by the operator P.

It is very important that the meaning of the operator P^* is *family-independent* since independent field variables are commutative with each other.* And the set of the independent field variables forms the defining system of the operator P^*.

An example of the use of this operator is

$$\begin{aligned}P^*[\dot{q}(t), q(t')]&=P^*\left[\lim_{\varepsilon\to0}\frac{q(t+\varepsilon)-q(t)}{\varepsilon},\ q(t')\right]\\&=\lim_{\varepsilon\to0}P\left[\frac{q(t+\varepsilon)-q(t)}{\varepsilon},\ q(t')\right]\\&=\frac{d}{dt}P[q(t), q(t')]\,.\end{aligned}\qquad (2\cdot12)^{**}$$

We shall remark here that the operator P^* is not always defined. In order that P^* can uniquely be defined, it is necessary to restrict the order of the poles of quantities appearing in the operand of the operator P^* to be lower than the order of the equations of motion of the independent field variables.

With this uniqueness condition, the properties a) and b) of the operator P are also satisfied by the operator P^*, but c) is not satisfied in general and somewhat modified.

c′) If the orders of the equations of motion of the independent field variables are finite, and if $t_1, t_2, \cdots$ are larger than $\tau_1, \tau_2, \cdots$ by finite amounts, then

$$\begin{aligned}&P^*[Q_1(t_1), Q_2(t_2), \cdots, R_1(\tau_1), R_2(\tau_2), \cdots]\\&\quad=P^*[Q_1(t_1), Q_2(t_2), \cdots]\cdot P^*[R_1(\tau_1), R_2(\tau_2)\cdots]\,.\end{aligned}$$

c″) If Q's are either monopole or dipole quantities, then

$$P^*[Q(t), Q'(t-0)]=Q(t)Q'(t-0),$$

because of the separability condition.

For instance,

$$P^*[\dot{q}(t), \dot{q}(t-0)]=\lim_{\varepsilon\to0}\frac{1}{\varepsilon^2}P[q(t+\varepsilon)-q(t), q(t)-q(t-\varepsilon)]$$

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* For Fermion fields we shall be concerned with such expressions that they occur in bilinear forms.

** In the case $t=t'$, we distinguish t' from t, and put t' equal to t only after the differentiation.

$$=\lim_{\varepsilon\to 0}\frac{q(t+\varepsilon)-q(t)}{\varepsilon}\cdot\frac{q(t)-q(t-\varepsilon)}{\varepsilon}=\dot{q}(t)\,\dot{q}(t-0).$$

where we put all infinitesimal quantities equal to ε, corresponding to Feynman's path integral.

§ 3. Transformation functions

In this section we shall construct transformation functions on the Lagrangian formalism.

The transformation function in the Hamiltonian formalism is, as was shown in the previous section, given by

$$U(t,\,t_0)=P[\exp\{-i\int_{t_0}^{t}H(t)dt\}]\,. \tag{3·1}$$

We shall show that in the Lagrangian formalism it is given by

$$U(t,\,t_0)=P^*[\exp\{i\int_{t_0}^{t}L(t)\,dt\}]\,. \tag{3·2}$$

Written in the covariant form, they become respectively

$$U(\sigma,\,\sigma_0)=P[\exp\{-i\int_{\sigma_0}^{\sigma}H(x)\,(dx)\}]\,, \tag{3·3}$$

$$U(\sigma,\,\sigma_0)=P^*[\exp\{i\int_{\sigma_0}^{\sigma}L(x)\,(dx)\}]\,, \tag{3·4}$$

in which H and L are Hamiltonian and Lagrangian densities.

Since the operator P^* in (3·4) has a definite meaning under the uniqueness condition and L is a world scalar function of only space-time coordinates not depending on the choice of the family of space-like surfaces, the transformation function in the expression (3·4) is uniquely determined by fixing two space-like surfaces σ and σ_0.

Both U's in (3·3) and (3·4) satisfy the same initial condition :

$$U(\sigma_0,\,\sigma_0)=1\,, \tag{3·5}$$

and the functional U in (3·3) satisfies the Tomonaga–Schwinger equation :

$$i\frac{\delta}{\delta\sigma(x)}U(\sigma,\,\sigma_0)=H(x)U(\sigma,\,\sigma_0)\,. \tag{3·6}$$

Thus for the proof of the equivalence of the expression (3·4) to (3·3), we have only to show that the Lagrangian transformation function (3·4) also satisfies the Tomonaga–Schwinger equation.

We shall assume hereafter that L involves only monopole and dipole quantities, i. e., the separability condition is fulfilled.

We shall now differentiate (3·4) with respect to the surface σ. Suppose that σ is deformed into σ' by an infinitesimal volume $d\Omega$, then

$$U(\sigma', \sigma_0) - U(\sigma, \sigma_0)$$
$$= P^*[\exp(i\int_{\sigma_0}^{\sigma'} L(x)\,(dx)) - \exp(i\int_{\sigma_0}^{\sigma} L(x)\,(dx))]$$
$$= P^*[\{\exp(i\int_{\sigma}^{\sigma'} L(x)\,(dx)) - 1\} \cdot \exp(i\int_{\sigma_0}^{\sigma} L(x)\,(dx))]\,.$$

The separability condition is of help to change the above expression into

$$U(\sigma', \sigma) - U(\sigma, \sigma_0) = P^*[\exp(i\int_{\sigma_0}^{\sigma} L(x)\,(dx)) - 1] \cdot U(\sigma, \sigma_0).$$

Put

$$\bar{H}(x) \equiv \frac{i}{d\Omega} P^*[\exp(i\int_{\sigma}^{\sigma'} L(x)\,(dx)) - 1]\,,$$

then it is necessary and sufficient for the proof of equivalence that the following equality holds :

$$\bar{H}(x) = H(x). \tag{3·8}$$

Since the transformation function (3·4) is uniquely determined by fixing two space-like surfaces σ and σ_0, the so-called integrability condition must be satisfied by $\bar{H}(x)$:

$$\left[i\frac{\delta}{\delta\sigma(x)} - \bar{H}(x),\ i\frac{\delta}{\delta\sigma(x')} - \bar{H}(x')\right]$$
$$= i\left(\frac{\delta\bar{H}(x)}{\delta\sigma(x')} - \frac{\delta\bar{H}(x')}{\delta\sigma(x)}\right) + [\bar{H}(x),\ \bar{H}(x')] = 0\,. \tag{3·9}$$
$$(x, x' \text{ on } \sigma)$$

The expansion of $\bar{H}(x)$ yields

$$\bar{H}(x) = \sum_{n=1}^{\infty} \frac{i^{n+1}}{n!} \cdot \frac{1}{d\Omega} \int_{\sigma}^{\sigma'} (dx_1) \cdots \int_{\sigma}^{\sigma'} (dx_n) P^*[L(x_1), \cdots, L(x_n)]\,. \tag{3·10}$$

The first term of this expansion is equal to

$$-L(x). \tag{3·11}$$

We shall give complete proofs for separate cases.

(I) *Case of free Bose fields*

Without loss of generality, we shall illustrate the proof by the neutral scalar field. The Lagrangian density of this field is given by

$$L_f = -\frac{1}{2}\left\{\left(\frac{\partial\phi}{\partial x_\mu}\right)^2 + \varkappa^2\phi^2\right\}. \tag{3·12}$$

The first term of the expansion of $\bar{H}_f$ is thus equal to $-L_f$, and remaining terms are expressed by

$$\frac{i^{n+1}}{n!} \cdot \frac{1}{d\Omega} \int_{\sigma}^{\sigma'} (dx_1) \cdots \int_{\sigma}^{\sigma'} (dx_n) P^*(L_f(x_1) \cdots L_f(x_n)). \quad (n > 1) \tag{3·13}$$

Since this expansion is an n-fold integral over an infinitesimal volume $d\Omega$, divided by $d\Omega$, the occurence of $(n-1)$ δ functions is required for the expression to survive.

Therefore we must at least $(n-1)$ times contract the wave functions to bring about the derivatives of Δ_F-function which effectively contain the δ-function.

We need not contract more than $(n-1)$ times, because the contribution from terms with more contractions are involved in those with less contractions.

Remember

$$\langle P(\phi(x), \phi(x'))\rangle_0 = \frac{1}{2}\Delta_F(x-x'), \tag{3·14}$$

and

$$(\Box^2 - \varkappa^2)\Delta_F(x-x') = 2i\delta(x-x'), \tag{3·15}$$

then we can easily understand that only contractions of dipole quantities produce δ-functions, and therefore for $n>1$ the expression (3·13) is also written as

$$\frac{i^{n+1}}{n!}\left(-\frac{1}{2}\right)^n \frac{1}{d\Omega}\int_\sigma^{\sigma'}(dx_1)\cdots\int_\sigma^{\sigma'}(dx_n)P^*\left[\left(\frac{\partial\phi}{\partial x_\mu}\right)^2(x_1), \cdots, \left(\frac{\partial\phi}{\partial x_\mu}\right)^2(x_n)\right], \tag{3·16}$$

for which we shall perform $(n-1)$ times contractions.

Since the domain enclosed with two space-like surfaces σ and σ' is an infinitesimal thin layer, the relation (3·15) may effectively be written as

$$\frac{\partial^2}{\partial x_\mu \partial x_\nu}\Delta_F(x-x') \approx -2i n_\mu n_\nu \delta(x-x'), \tag{3·17}$$

where n_μ is the unit normal to the surface σ at the point x.

From the above argument, it is clear that $\bar{H}_f$ must be of the form as

$$\bar{H}_f = -L_f + a\frac{\partial\phi}{\partial x_\mu}\cdot\frac{\partial\phi}{\partial x_\nu}n_\mu n_\nu,$$

where a is a numerical factor. The constant a is determined by the condition (3·9), which yields the desired relation:

$$\begin{aligned}\bar{H}_f &= -L_f + \frac{\partial\phi}{\partial x_\mu}\cdot\frac{\partial\phi}{\partial x_\nu}\cdot n_\mu n_\nu \\ &= -L_f + \frac{\partial L_f}{\partial(\partial\phi/\partial x_\mu)}\cdot\frac{\partial\phi}{\partial x_\nu}n_\mu n_\nu = H_f .\end{aligned} \tag{3·18}$$

The direct method to compute $\bar{H}_f$ from (3·10) fails because of the lack of convergence.

(II) *Case of free Fermi fields*

The Fermi fields obey first order differential equations, so that we cannot attach a definite meaning to the operator P^* if the derivatives of the wave functions occur in the operand.

Thus the expression (3·2) or (3·4) is meaningless in this case.

In the Feynman theory also, the path integral could not be defined for Dirac fields because of the lack of any classical analogue, hence he started from the fact that the

transformation functions for free fields can be treated as Green functions in other definite cases.[5]

At any rate, the application of Lagrangian method to free fields does not seem to be a good subject. Its utility consists in the application to interacting fields.

(III) *Case of interacting fields*

We shall treat the case of interacting fields, and for this purpose we employ the interaction representation.

Then

$$\bar{H}_{\text{int}}(x)=\frac{i}{d\Omega}P^*[\exp\{i\int_{\sigma}^{\sigma'}L_{\text{int}}(x)(dx)\}-1],\quad (d\Omega\to 0). \tag{3·19}$$

We assume here that L_{int} involves dipole quantities at most linearly, then in the expansion of (3·19) only first two terms survive, i. e.

$$\bar{H}_{\text{int}}(x)=-L_{\text{int}}(x)-\frac{i}{2}\frac{1}{d\Omega}\int_{\sigma}^{\sigma'}(dx')\int_{\sigma}^{\sigma'}(dx'')P^*(L_{\text{int}}(x'),L_{\text{int}}(x'')). \tag{3·20}$$

The second term survives only if two dipole quantities with different arguments are contracted so as to produce the δ–function.

The only possible dipole quantities are the derivatives of the Boson wave functions because of the uniqueness condition. We shall denote the independent variables of Bosons by Q_α, $Q_\beta{}^*$, then we see

$$[Q_\alpha(x),Q_\beta{}^*(x')]=i\delta_{\alpha\beta}\Delta(x-x'). \tag{3·21}$$

From the contraction of dipole quantities follows

$$\begin{aligned}\bar{H}_{\text{int}}(x)=&-L_{\text{int}}(x)-\frac{i}{2}\frac{1}{d\Omega}\int_{\sigma}^{\sigma'}(dx')\int_{\sigma}^{\sigma'}(dx'')\left\langle P^*\left(\frac{\partial Q_\alpha'}{\partial x_\mu'},\frac{\partial Q_\beta^{*\prime\prime}}{\partial x_\nu''}\right)\right\rangle_0\\&\times P^*\left(\frac{\partial L_{\text{int}}'}{\partial(\partial Q_\alpha'/\partial x_\mu')}\cdot\frac{\partial L_{\text{int}}''}{\partial(\partial Q_\beta^{*\prime\prime}/\partial x_\nu'')}\right)\\&+\text{terms with } Q \text{ and } Q^* \text{ interchanged and of neutral fields.}\end{aligned} \tag{3·22}$$

In evaluating the above expression, we must remember

$$\begin{aligned}\left\langle P^*\left(\frac{\partial Q_\alpha'}{\partial x_\mu'},\frac{\partial Q_\beta^{*\prime\prime}}{\partial x_\nu''}\right)\right\rangle_0&=\delta_{\alpha\beta}\frac{\partial^2}{\partial x_\mu'\partial x_\nu''}\left(\frac{1}{2}\Delta_F(x'-x'')\right)\\&\approx i\delta_{\alpha\beta}n_\mu n_\nu\delta(x'-x''),\quad\text{(effectively)}\end{aligned}$$

and

$$P^*\left(\frac{\partial L_{\text{int}}'}{\partial(\partial Q_\alpha'/\partial x_\mu')}\cdot\frac{\partial L_{\text{int}}''}{\partial(\partial Q_\beta^{*\prime\prime}/\partial x_\nu'')}\right)=P(\quad,\quad),$$

since there is no dipole quantity in the operand.

The following relation is also utilized:

$$\lim_{t'\to t}P(A(t)B(t')+B(t)A(t'))=A(t)B(t)+B(t)A(t).$$

With the help of these relations, the equation (3·22) becomes

$$\bar{H}_{\rm int}(x)=-L_{\rm int}(x)$$
$$+\frac{1}{2}n_\mu n_\nu\Big[\frac{\partial L_{\rm int}}{\partial(\partial Q_\alpha/\partial x_\mu)}\cdot\frac{\partial L_{\rm int}}{\partial(\partial Q_\alpha^*/\partial x_\nu)}+\frac{\partial L_{\rm int}}{\partial(\partial Q_\alpha^*/\partial x_\mu)}$$
$$\times\frac{\partial L_{\rm int}}{\partial(\partial Q_\alpha/\partial x_\nu)}+\frac{\partial L_{\rm int}}{\partial(\partial Q_\alpha{}^0/\partial x_\mu)}\cdot\frac{\partial L_{\rm int}}{\partial(\partial Q_\alpha{}^0/\partial x_\nu)}\Big]. \qquad (3\cdot23)$$

That $\bar{H}_{\rm int}(x)$ fulfills the requirement of the integrability condition is obvious from the general argument.

Next we must derive $H_{\rm int}(x)$ from the canonical theory.

The total Lagrangian density consists of free and interaction Lagrangian densities:

$$L_{tot}=L_f+L_{\rm int}. \qquad (3\cdot24)$$

Our problem is to find $H_{\rm int}$ in the interaction representation. The canonical conjugate variables to Q_α are

$$L_f\to P_\alpha=\frac{\partial L_f}{\partial\dot{Q}_\alpha}, \qquad \text{(free case)}$$
$$L_{tot}\to P_\alpha{}^*=P_\alpha+\frac{\partial L_{\rm int}}{\partial\dot{Q}_\alpha}, \qquad \text{(interacting case)} \qquad (3\cdot25)$$

and the interaction Hamiltonian is given by

$$H_{\rm int}=H_{tot}(P^*,\,Q)-H_f(P^*,\,Q). \qquad (3\cdot26)$$

We shall express H_f as functions of P and Q, instead of P^* and Q, then

$$H_{tot}=P_\alpha{}^*\dot{Q}_\alpha-L_{tot}(P,\,Q)$$
$$=P_\alpha\dot{Q}_\alpha-L_f(P,\,Q)-L_{\rm int}(P,\,Q)+\dot{Q}_\alpha(P_\alpha{}^*-P_\alpha)$$
$$=H_f(P,\,Q)-L_{\rm int}(P,\,Q)+\dot{Q}_\alpha(P_\alpha{}^*-P_\alpha).$$

While

$$H_f(P,\,Q)=H_f(P^*,\,Q)+\frac{\partial H_f}{\partial P_\alpha}(P_\alpha-P_\alpha{}^*)+\frac{1}{2}\frac{\partial^2 H_f}{\partial P_\alpha\partial P_\beta}(P_\alpha-P_\alpha{}^*)(P_\beta-P_\beta{}^*),$$

and in the interaction representation holds

$$\frac{\partial H_f}{\partial P_\alpha}=\dot{Q}_\alpha,$$

Hence

$$H_{tot}=H_f(P^*,\,Q)-L_{\rm int}(P,\,Q)+\frac{1}{2}\frac{\partial^2 H_f}{\partial P_\alpha\partial P_\beta}(P_\alpha-P_\alpha{}^*)(P_\beta-P_\beta{}^*). \qquad (3\cdot27)$$

Reexpressing $L_{\rm int}(P,\,Q)$ as functions of P^* and Q, and then replacing P^* by P, we have

$$H_{\rm int}=-L_{\rm int}+\frac{1}{2}\frac{\partial^2 H_f}{\partial P_\alpha\partial P_\beta}(P_\alpha-P_\alpha{}^*)(P_\beta-P_\beta{}^*). \qquad (3\cdot28)$$

Combining (3·25) and (3·28), we finally arrive at

$$H_{\text{int}}=-L_{\text{int}}+\frac{1}{2}\left[\frac{\partial L_{\text{int}}}{\partial \dot{Q}_\alpha}\cdot\frac{\partial L_{\text{int}}}{\partial \dot{Q}_\alpha{}^*}+\frac{\partial L_{\text{int}}}{\partial \dot{Q}_\alpha{}^*}\cdot\frac{\partial L_{\text{int}}}{\partial \dot{Q}_\alpha}+\frac{\partial L_{\text{int}}}{\partial \dot{Q}_x{}^0}\cdot\frac{\partial L_{\text{int}}}{\partial \dot{Q}_\alpha{}^0}\right].$$

If we replace the time derivatives by the normal component of the gradient, there follows at once the equality

$$\bar{H}_{\text{int}}=H_{\text{int}}\,.$$

§ 4. Commutation relations via Heisenberg operators

Although the interaction representation is convenient to construct transformation functions, we have to refer to the Heisenberg representation in the calculation of the expectation values of operators, so that several authors have investigated Heisenberg operators.[6]

We shall, however, utilize the Heisenberg operators only to derive commutation relations based on the Yang-Feldman formalism[4] and Peierls' idea.[7] We shall denote operators in the Heisenberg and interaction representations by thick and thin letters respectively.

There are two ways to derive the equations of motion of Heisenberg operators. The one is to bring the free operators (operators in the interaction representation) into play, i. e. to express Heisenberg operators by

(a) $$\boldsymbol{Q}_\alpha(x/\sigma)=U(\sigma,\sigma_0)^{-1}Q_\alpha(x)U(\sigma,\sigma_0),\quad (x \text{ on } \sigma) \qquad (4\cdot1)^*$$

then we can trace the motion of $\boldsymbol{Q}(x/\sigma)$ on the information about the free operators. The other is to refer to the variation principle, i. e. to derive equations of motion from

(b) $$\delta\int \boldsymbol{L}_{t_0\sigma}(dx)=0\,. \qquad (4\cdot2)$$

In the former case, we need to know commutation relations of free operators, while in the latter case we need not.

This difference suggests us that the comparison of the two methods will lead us to commutation relations as the *necessary condition* for the two methods to give the same results. From such a point of view, we shall investigate the commutation relations.

For this purpose we shall assume that the interaction is adiabatically switched on in the remote past and switched off again adiabatically in the remote future. This hypothesis is harmless for the investigation of such relations.

Thus at $t=-\infty$, the Heisenberg operators become identical with the free operators, and we shall call the free fields at $t=-\infty$ as incoming fields; similarly outgoing fields are defined at $t=+\infty$.

With this nomenclature, the Heisenberg operators are written by the method (a) as

$$\boldsymbol{Q}_\alpha(x)=U(\sigma,-\infty)^{-1}Q_\alpha^{\text{in}}(x)U(\sigma,-\infty). \qquad (4\cdot3)$$

The relation of the outgoing fields to incoming fields is, as is well known, (See Appendix)

$$Q_\alpha^{\text{out}}(x)=S^{-1}Q_\alpha^{\text{in}}(x)S\,. \qquad (4\cdot4)$$

We shall expand $(4\cdot3)$, and shall write explicitly to the first order in the interaction Lagrangian

* We assume Q's to be monopole quantities.

$$\text{(a)} \qquad \boldsymbol{Q}_\alpha(x) = Q_\alpha^{\text{in}}(x) - i\int_{-\infty}^{\sigma} [L_{\text{int}}(x'),\, Q_\alpha^{\text{in}}(x)](dx') + \cdots . \tag{4·5}$$

Next we shall relate the expansion to the variation principle, i. e. to the method (b).

The variation principle is

$$\delta \int (\boldsymbol{L}_f + \boldsymbol{L}_{\text{int}})(dx) = 0 . \tag{4·6}$$

In order to study the incoming fields, we may omit $\boldsymbol{L}_{\text{int}}$ at $t = -\infty$, then the equations of motion of the incoming fields are derived from

$$\delta \int L_f(dx) = 0 . \tag{4·7}$$

For instance, the equation of motion of Q^{in} is

$$\frac{\delta L_f}{\delta Q_\alpha{}^*} = 0 \qquad \text{or} \quad D_{\alpha\beta}(\partial) Q_\beta^{\text{in}} = 0 , \tag{4·8}$$

where Q^* is the hermitian conjugate of Q and $D_{\alpha\beta}(\partial)$ some differential operator, and

$$\frac{\delta}{\delta Q} = \frac{\partial}{\partial Q} - \frac{\partial}{\partial x_\mu} \cdot \frac{\partial}{\partial (\partial Q / \partial x_\mu)} .$$

While the general Heisenberg operators obey the equations :

$$\frac{\delta \boldsymbol{L}_f}{\delta \boldsymbol{Q}_\alpha{}^*} = -\frac{\delta \boldsymbol{L}_{\text{int}}}{\delta \boldsymbol{Q}_\alpha{}^*} \quad \text{or} \quad D_{\alpha\beta}(\partial) \boldsymbol{Q}_\beta = -\frac{\delta \boldsymbol{L}_{\text{int}}}{\delta \boldsymbol{Q}_\alpha{}^*} . \tag{4·9}$$

We shall solve the equation (4·9) with the initial condition :

$$\boldsymbol{Q}_\beta = Q_\beta^{\text{in}} \quad \text{at} \quad t = -\infty .$$

For convenience, the Green functions for the incoming fields are introduced as

$$\begin{aligned} &D_{\alpha\beta}(\partial) G_{\beta\gamma}^{\text{ret}}(x - x') = \delta_{\alpha\gamma} \delta(x - x'), \\ &G_{\beta\gamma}^{\text{ret}}(x - x') = 0 \quad \text{for} \quad t - t' < 0. \end{aligned} \tag{4·10}$$

We shall assume the existence of such Green functions for the time being, then the equation (4·9) is changed into the following integral equation

$$\boldsymbol{Q}_\alpha(x) = Q_\alpha^{\text{in}}(x) - \int_{-\infty}^{\sigma} (dx')\, G_{\alpha\beta}^{\text{ret}}(x - x') \frac{\delta \boldsymbol{L}_{\text{int}}(x')}{\delta \boldsymbol{Q}_\beta{}^*(x')} . \tag{4·11}$$

This equation can formally be solved by successive substitutions, and we shall write to the first order in the interaction Lagrangian

$$\text{(b)} \qquad \boldsymbol{Q}_\alpha(x) = Q_\alpha^{\text{in}}(x) - \int_{-\infty}^{\sigma} (dx')\, G_{\alpha\beta}^{\text{ret}}(x - x') \frac{\delta L_{\text{int}}(x')}{\delta Q_\beta^{*\text{in}}(x')} + \cdots . \tag{4·12}$$

In order that the two methods give the same results, we have to admit the equality

$$-i\int_{-\infty}^{\sigma} [L_{\text{int}}(x'),\, Q_\alpha^{\text{in}}(x)](dx') = -\int_{-\infty}^{\sigma} (dx')\, G_{\alpha\beta}^{\text{ret}}(x - x') \frac{\delta L_{\text{int}}(x')}{\delta Q_\beta^{*\text{in}}(x')} . \tag{4·13}$$

Equating the integrands of both sides, we have

$$[Q_\alpha^{\text{in}}(x), L_{\text{int}}(x')] = i G_{\alpha\beta}^{\text{ret}}(x - x') \frac{\delta L_{\text{int}}}{\delta Q_\beta^{*\text{in}}}(x'), \quad \text{for} \quad t > t', \tag{4·14}$$

where L_{int} is expressed in terms of incoming fields.

Quite analogously to the above procedure, we can also start from the advanced solutions. With the final condition:

$$Q_\beta = Q_\beta^{\text{out}} \quad \text{at} \quad t = +\infty,$$

we find

$$[Q_\alpha^{\text{out}}(x), L_{\text{int}}(x')] = -iG_{\alpha\beta}^{\text{adv}}(x-x')\frac{\delta L_{\text{int}}}{\delta Q_\beta^{*\text{out}}}(x'), \quad \text{for} \quad t<t', \tag{4·15}$$

where L_{int} is expressed in terms of outgoing fields, and

$$D_{\alpha\beta}(\partial)G_{\beta\gamma}^{\text{adv}}(x-x') = \delta_{\alpha\gamma}\delta(x-x'),$$
$$G_{\beta\gamma}^{\text{adv}}(x-x') = 0 \quad \text{for} \quad t-t'>0\,. \tag{4·16}$$

Since incoming fields and outgoing fields are connected by a unitary transformation S, they must satisfy the same commutation relations, so that we can omit the subscripts *in* and *out* to express commutation relations in the interaction representation.

Then synthesizing (4·14) and (4·15), we have

$$[Q_\alpha(x), L_{\text{int}}(x')] = iG_{\alpha\beta}(x-x')\frac{\delta L_{\text{int}}}{\delta Q_\beta^*}(x'), \tag{4·17}$$

where

$$G(x) = -(G^{\text{adv}}(x) - G^{\text{ret}}(x)) = \begin{cases} G^{\text{ret}}(x), & \text{for } t>0\,, \\ -G^{\text{adv}}(x), & \text{for } t<0\,. \end{cases}$$

Now if Q is the wave function of a field with integral spin, then there can be such interaction Lagrangians that involve the wave functions Q and Q^* only linearly, for which we obtain only $(-)$-type commutation relations, i. e.

$$[Q_\alpha(x), Q_\beta^*(x')] = iG_{\alpha\beta}(x-x'). \tag{4·18}$$

Thus fields with integral spin obey the Bose-Einstein statistics. If on the other hand, Q is the wave function of a field with half-integral spin, then there can be only such interaction Lagrangians that involve Q^* always accompanied with its conjugate function Q or the wave function of other spinor fields.

In this case, we reach two possibilities:

(1) $\{Q_\alpha(x), Q_\beta^*(x')\} = iG_{\alpha\beta}(x-x')$,
and others anticommute.

(2) $[Q_\alpha(x), Q_\beta^*(x')] = iG_{\alpha\beta}(x-x')$,
and others commute.

However, in order to avoid the negative energy difficulty by the exclusion principle, we should choose the former case.[8]

Thus fields with half-integral spin obey the Fermi-Dirac statistics.

Appendix

The relation of the outgoing fields to the incoming fields.

In the text, we have imposed superfluous boundary conditions on the Heisenberg operators, i. e.

(1) $\quad \boldsymbol{Q}_\beta = Q_\beta^{\text{in}} \quad$ at $\quad t=-\infty \quad$ (initial condition),

(2) $\quad \boldsymbol{Q}_\beta = Q_\beta^{\text{out}} \quad$ at $\quad t=+\infty \quad$ (final condition).

Only one of these two conditions is necessary and sufficient, so that the incoming fields and outgoing fields must be expressed in terms of alternative fields.

From the initial condition,

$$\boldsymbol{Q}(x) = U^{\text{in}}(\sigma, -\infty)^{-1} Q^{\text{in}}(x) U^{\text{in}}(\sigma, -\infty),$$

where

$$U^{\text{in}}(\sigma, -\infty) = P^*[\exp(i \int_{-\infty}^{\sigma} L_{\text{int}}^{\text{in}}(x)(dx))].$$

From the final condition, follows

$$Q^{\text{out}}(x) = (S^{\text{in}})^{-1} Q^{\text{in}}(x) S^{\text{in}}, \quad S^{\text{in}} = U^{\text{in}}(\infty, -\infty).$$

By this relation, it is easily seen that

$$S^{\text{out}} = P^*[\exp(i \int_{-\infty}^{\infty} L_{\text{int}}^{\text{out}}(x)(dx))]$$

$$= (S^{\text{in}})^{-1} \cdot P^*[\exp(i \int_{-\infty}^{\infty} L_{\text{int}}^{\text{in}}(x)(dx))] \cdot S^{\text{in}} = S^{\text{in}} \equiv S.$$

With the help of these relations, we get

$$\boldsymbol{Q}(x) = U^{\text{in}}(\sigma, -\infty)^{-1} Q^{\text{in}}(x) U^{\text{in}}(\sigma, -\infty)$$
$$= U^{\text{out}}(\infty, \sigma) Q^{\text{out}}(x) U^{\text{out}}(\infty, \sigma)^{-1},$$

which was already implicitly used to derive the equation (4·15).

Note added in proof

1) In deriving (4·14) from (4·13), the results are not unique and we also have

$$[Q_\alpha^{\text{in}}(x), L_{\text{int}}(x')] = i\Big(\frac{\partial L'_{\text{int}}}{\partial Q_\beta^{*\text{in}}} + \frac{\partial L'_{\text{int}}}{\partial(\partial Q_\beta^{*\text{in}}/\partial x_\mu')} \cdot \frac{\partial}{\partial x_\mu'}\Big) G_{\alpha\beta}^{\text{ret}}(x-x'), \quad \text{for} \quad t > t',$$

by partial integration, and it is this form of equality that enables us to derive consistent C. R.'s rather than (4·14). The partial integration is allowed only within the frame of canonical formalism.

2) Although the procedure to construct C. R.'s are proved only for the monopole quantities, the results are also applicable to general field variables, which we shall prove here. The field variables $\mathfrak{Q}$'s can be expressed as the linear combination of the monopoles Q's:

$$\mathfrak{Q}_A = d_{A\alpha} Q_\alpha, \quad (A=1, 2, \cdots, F;\ \alpha=1, 2, \cdots, f), \qquad \text{(A·1)}$$

where the coefficients d's are generally differential operators.

Then

$$[\mathfrak{Q}_A(x), \mathfrak{Q}_B^*(x')]_{\pm}=i\mathfrak{G}_{AB}(x-x'), \quad \mathfrak{G}_{AB}^{(\ )}=d_{A\alpha}\tilde{d}_{B\beta}^* G_{\alpha\beta}^{(\ )}, \tag{A·2}$$

where * denotes complex conjugation and $\sim$ to change the sign of each differential.

Put

$$\delta L_f/\delta Q_\alpha^*=D_{\alpha\beta}(\partial)Q_\beta \quad \text{and} \quad \delta L_f/\delta \mathfrak{Q}_A^*=\mathfrak{D}_{AB}(\partial)\mathfrak{Q}_B, \tag{A·3}$$

then from (A·1) and (A·3), we readily see

$$D_{\alpha\beta}=\tilde{d}_{A\alpha}^*\mathfrak{D}_{AB}d_{B\beta}. \tag{A·4}$$

Combining (A·2), (A·4) and (4·10), we get

$$\tilde{d}_{A\alpha}^*[\mathfrak{D}_{AB}\mathfrak{G}_{BC}^{\mathrm{ret}}(x-x')-\delta_{AC}\cdot\delta(x-x')]=0,$$

from which follows at once

$$\mathfrak{D}_{AB}\mathfrak{G}_{BC}^{\mathrm{ret}}(x-x')=\delta_{AC}\cdot\delta(x-x'), \tag{A·5}$$

provided that $f\geq F$, e. g. Stückelberg formalism for vector meson.

If, on the contrary, $f\leq F$, e. g. elimination of the fourth component for the vector meson, we can prove (4·10) starting from (A·5) in a similar way to the above proof. Thus quantities related to monopoles are completely eliminated.

We also have

$$\mathfrak{D}_{AB}\langle P^*(\mathfrak{Q}_B(x), \mathfrak{Q}_C^*(x'))\rangle_0=i\delta_{AC}\cdot\delta(x-x'), \tag{A·6}$$

effectively within the frame of canonical formalism.

In the above expression, we may have to better replace the symbol P^* by an analogous symbol T^*.

References

1) F. J. Dyson, Phys. Rev. **75** (1949), 486.
   Also see R. P. Feynman, Phys. Rev. **84** (1951), 108.
2) R. P. Feynman, Rev. Mod. Phys. **20** (1948), 367; Phys. Rev. **80** (1950), 440.
3) Y. Nambu, Prog. Theor. Phys. **7** (1952), 131.
4) Z. Koba, Prog. Theor. Phys. **5** (1950), 696.
   K. Nishijima, Prog. Theor. Phys. **5** (1950), 405, 813.
   There are serious mistakes in the content of the latter paper, which are corrected in the present paper.
   Y. Nambu, see ref. (3).
5) R. P. Feynman, Phys. Rev. **76** (1949), 749, 769.
6) C. N. Yang and D. Feldman, Phys. Rev. **79** (1950), 972.
   G. Källen. Arkiv för Fysik, Bd. 2, Nr. 19, (1950).
   F. J. Dyson, Phys. Rev. **82** (1951), 428; **83** (1951), 608.
7) R. E. Peierls, to be published.
   The author wishes to express his thanks to Prof. Peierls for having made him available his paper in advance of publication.
8) W. Pauli, Phys. Rev. **58** (1940), 716.

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On the Magnetism of Magnetic Compounds

—— *General Treatment of Superexchange Interaction* ——

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In this paper the theories of superexchange interaction developed by Kramers and Anderson have been more generally reformalized by means of the well-known vector model. The formulation can also be applied to the problem of molecular structure in which a consideration of the various orbital configurations of electrons is required. From an application of this method to the crystal which contains the magnetic ions separated from each other by the negative ions, it is found that magnetic interaction (or superexchange interaction), can be written in terms of spin operators as well as the ordinary exchange interaction, as Anderson concluded previously. As far as one accepts the assumptions that interatomic exchange integrals are negative and inneratomic exchange integrals positive, it must be said that superexchange interaction is ferromagnetic if one considers only the intermediate states in which an electron on a negative ion has jumped into an unoccupied orbit of the neighbouring magnetic ion. On the other hand the superexchange interaction is antiferromagnetic if one considers only the intermediate states in which the electron has jumped into the orbit which is already occupied by an electron. Actually two sorts of these interactions will be considered to be co-existent in any magnetic compounds and the antiferromagnetic coupling seems to be predominant in most cases.

§ 1. Introduction

From the recent experiments of the neutron diffraction about the various antiferromagnetic compounds performed by Shull and his coworkers,[1] it has been found that the magnetic interaction between the magnetic ions which are separated from each other by negative non-magnetic ions is more important than the interaction between those which are immediate neighbours. And also from the interpretations of the temperature dependences of susceptibilities in many antiferromagnetic compounds, it has been suggested that this sort of magnetic interaction must also be considered.[2,3]

In accord with these experimental facts, Anderson[4] has shown that the superexchange interaction which was first proposed by Kramers[5] can be written down in terms of spin operators; and the directional property of this interaction can be explained by the symmetrical distribution of the p orbits in a negative ion.

Now for the sake of simplicity we take MnO as an example and assume that this crystal is completely ionic in its ground state. Then the ordinary exchange spin-coupling between the Mn ions separated from each other by negative ions (between next nearest neighbours) is usually considered to be absent. According to Kramers' mechanism, however, if we consider the excited state of the crystal that an electron on an O^{--} ion has

been translated to an orbit of its adjacent Mn^{++} ion and the remaining negative ion becomes paramagnetic, and admix these excited states to the ground state in a certain proportion, we can expect to obtain the spin-coupling between the Mn ions which are intermediated by the negative ions.

Kramers treated these excited configurations as perturbations to the ground configuration and showed that the superexchange interaction is expressed by the third-order perturbing terms. Anderson has reduced Kramers' formula to the ordinary expression of the spin-coupling where he has taken into account the spin-coupling in a magnetic ion to be considerably strong. In the case where an electron on a negative ion has gone to an unoccupied orbit of a magnetic ion and the internal exchange splittings in the magnetic ion are as large as the ground-excited orbital splitting which the transition electron receives, the energy of a certain spin state of the excited configuration may be lower than that of the ground configuration so that the perturbational treatment will be unsuitable for the calculation of the superexchange interaction. But in the case where an electron on a negative ion has gone to the level of a magnetic ion which is already occupied by an electron, the inner exchange interaction in the magnetic ion disappears strictly on account of the Pauli principle and the perturbational treatment will remain useful.

Then in order to calculate the superexchange interaction without regarding the inner exchange interaction as a perturbing term, there will be no way for the present but to calculate the energies of every spin state by means of Serber's method,[6] taking a simple model as shown in the Appendix. In the present paper we calculate the superexchange interaction in a linear lattice regarding the internal exchange interaction in a magnetic ion as perturbations.

According to another conclusion of Anderson,[4] the superexchange interaction between two magnetic ions with more than half-filled $3d$ shells has been found to be antiferromagnetic and that between two magnetic ions with less than half-filled $3d$ shells has been found to be ferromagnetic. The former case is completely compatible with many experimental facts. The latter case, however, is not necessarily so, because the manganites, especially the ones that contain divalent metal ions ($CaMnO_3$ etc.), have been found to be likely antiferromagnetic by Jonker and van Santen,[7] Cr_2O_3 which has the same crystal structure with α–Fe_2O_3 is also antiferromagnetic[8] and MnO_2 and CrSb have been confirmed as antiferromagnetic substances by the neutron diffractions.[9]

In these compounds which contain the magnetic ions with less than half-filled $3d$ shells, we can obtain the antiferromagnetic spin-coupling if we consider the intermediate states that an electron has been translated from a negative ion to the orbit of the neighbouring magnetic ion which is already occupied by another electron. In spite of the disadvantage of the inner exchange energy in the magnetic ion this circumstance will be favourable if the splittings of $3d$ levels of the magnetic ions are caused by the surrounding crystal field, as Polder remarked.[10] On the other hand in the case of the magnetic ions with more than half-filled $3d$ shells, we shall be able to obtain the ferromagnetic spin-coupling too if we consider the intermediate states that an electron has jumped into an unoccupied orbital state, for example, the $4s$ orbit, of the adjacent magnetic ion. Then

in actual crystals one must ask for the superexchange interactions one by one examining the above-mentioned processes.

§ 2. Reformulation of Kramers' formula by the vector model

Before we discuss the superexchange interaction, we reformulate Kramers' formula in another way which is not essentially different. In the first place the total wave function of the N electron system in which the N electrons occupy independent orbits respectively will be constructed by means of the vector model so as to satisfy the Pauli principle.

Let the space co-ordinates and the spin co-ordinates of N electrons be $\boldsymbol{r}_1, \boldsymbol{r}_2, \cdots \boldsymbol{r}_N$ and $\xi_1, \xi_2, \cdots \xi_N$ respectively. The total wave function $\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \cdots \boldsymbol{r}_N; \xi_1, \xi_2, \cdots \xi_N)$ can be expanded by a complete and orthogonal set of spin functions, $\{\theta_k(\xi_1, \xi_2, \cdots \xi_N)\}$, $(k=1, 2, \cdots f)$, as follows:*

$$\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \cdots \boldsymbol{r}_N; \xi_1, \xi_2, \cdots \xi_N) = \sum_{k=1}^{f} \psi_k(\boldsymbol{r}_1, \boldsymbol{r}_2, \cdots \boldsymbol{r}_N)\, \theta_k(\xi_1, \xi_2, \cdots \xi_N). \qquad (1)$$

If a certain permutation which is denoted by P on the space co-ordinates and P^σ on the spin co-ordinates of the N electron system operates on the wave function Ψ, owing to the Pauli principle it must be held that

$$\varepsilon_p \Psi = \sum_k P\psi_k(\boldsymbol{r}_1, \boldsymbol{r}_2, \cdots \boldsymbol{r}_N)\, P^\sigma \theta_k(\xi_1, \xi_2, \cdots \xi_N), \qquad (2)$$

where $\varepsilon_p = +1$ if P is an even permutation or $\varepsilon_p = -1$ if P is an odd permutation. From Eqs. (1) and (2) and the orthogonality of θ_k, we have

$$\varepsilon_p \psi_{k'} = \sum_k P\psi_k P^\sigma_{k'k}, \qquad (3)$$

where

$$P^\sigma_{k'k} = \int \theta^*_{k'} P^\sigma \theta_k d\xi .$$

Now the set of the functions $\{\psi_k\}$ is approximated as usual by the function ψ that is determined by a certain orbital configuration of N electrons and is a product of one-electron wave functions. Since the function $Q\psi$, where Q is an arbitrary permutation, is thought to represent the same state as the original function ψ, ψ_k will be expanded on account of the fact that the N orbits are independent of each other as follows:

$$\psi_k = \sum_Q C_k(Q)\, Q\psi . \qquad (4)$$

From Eqs. (3) and (4) the coefficients $C_k(Q)$ must satisfy the following equations,

$$\varepsilon_p C_{k'}(Q) = \sum_k C_k(P^{-1}Q) P^\sigma_{k'k} . \qquad (5)$$

The permutation P in Eq. (5) is arbitrary so that if we choose P such as

$$P^{-1}Q = E, \quad \text{or} \quad P = Q,$$

Eq. (5) becomes

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* The set of spin functions, $\{\theta_k(\xi_1, \xi_2, \cdots \xi_N)\}$, is arbitrary for our purpose so long as it is complete and orthogonal.

$$\varepsilon_p C_{k'}(P) = \sum_k C_k(E) P^{\sigma}_{k'k} . \qquad (5')$$

Here as $C_k(E)$ can be arbitrarily taken we choose $C_k(E)$ as follows:

$$C_m(E) \neq 0, \; C_1(E) = C_2(E) = \cdots = C_f(E) = 0, \qquad (6)$$

where f is the total number of functions in the set $\{\theta_k\}$. Thus from Eq. (5′)

$$C_k(P) = a \varepsilon_p P^{\sigma}_{k,m} ,$$

where a is the constant which ought to be determined by the normalization of Φ.

Introduce the solutions of $C_k(P)$ into Eq. (4), and we have from Eq. (1) and the completeness of $\{\theta_k\}$, the following:

$$\Phi_m = a \sum_p \varepsilon_p P \psi P^{\sigma} \theta_m . \quad (m = 1, 2, \cdots f) \qquad (7)$$

This set of the total wave functions $\{\Phi_m\}$ is an orthogonal set in the spin space and satisfies the Pauli principle as all the one-electron orbital wave functions involved in ψ are orthogonal with each other.

So far we have considered only a single configuration of the N electron system, namely ψ, but hereafter we shall take together many configurations $\psi_t (t = 1, 2, \cdots)$, which are assumed to be orthogonal with each other and to be orthogonal with the original configuration or the ground configuration ψ_0. Then we make a linear combination of ψ_0 and ψ_t as

$$\psi = a\psi_0 + \sum_t C_t \psi_t . \qquad (8)$$

The total wave functions Φ_m, in which ψ is taken as Eq. (8), satisfy Schrödinger's equation:

$$H\Phi_m = W\Phi_m , \qquad (9)$$

where H is the total Hamiltonian of the N electron system and does not contain the term related to the spins.

As we do not intend to obtain the representation in spin space, the spin functions $\{\theta_m\}$ in Eq. (9) may be omitted and Eq. (9) will be rewritten as

$$H\Phi = W\Phi , \qquad (10)$$

where

$$\Phi = a \sum_p \varepsilon_p P \psi_0 P^{\sigma} + \sum_t C_t \sum_p \varepsilon_p P \psi_t P^{\sigma}, \qquad (11)$$

and the constant a in Eq. (7) and the normalization factor of Φ have been included in the coefficients a and C_t.

If Eq. (10) is multiplied by the complex conjugate of ψ_0 or ψ_t and integrated in the co-ordinate space of N electrons, we have from the orthogonality relations among ψ_0 and ψ_t, the following:

$$\begin{aligned} a(t_0 | H | t_0) + \sum_{t'} C_{t'}(t_0 | H | t') &= aW , \\ a(t | H | t_0) + \sum_{t'} C_{t'}(t | H | t') &= C_t W , \end{aligned} \qquad (12)$$

where

$$(t_0|H|t_0)=\sum_p \varepsilon_p P^\sigma \int \psi_0^* H P \psi_0 d\tau\,,$$

$$(t_0|H|t')=\sum_p \varepsilon_p P^\sigma \int \psi_0^* H P \psi_{t'} d\tau\,,$$

$$(t|H|t_0)=\sum_p \varepsilon_p P^\sigma \int \psi_t^* H P \psi_0 d\tau\,,$$

$$(t|H|t')=\sum_p \varepsilon_p P^\sigma \int \psi_t^* H P \psi_{t'} d\tau\,. \qquad (13)$$

The expressions in (12) are essentially equivalent to the one obtained by Serber's method[6] although the representation in spin space is not taken in (12). The secular equation in the latter method, however, becomes troublesome unless the system considered is composed of a few electrons, for example, the 4 electron system at most.

Like Kramers, we solve the formulas (12) by the method of perturbation assuming that $(t_0|H|t_0)=E_0$ is smaller than every $(t|H|t)$ and all non-diagonal elements, $(t_0|H|t')$, $(t|H|t')$, etc., are smaller than all diagonal elements, E_0 and $(t|H|t)$. Thus from the third-order approximation we obtain

$$C_t=\frac{a(t|H|t_0)}{E_0-(t|H|t)}+\sum_{t'\neq t}{}'\frac{a(t|H|t')(t'|H|t_0)}{\{E_0-(t'|H|t')\}\{E_0-(t|H|t)\}}$$
$$+\sum_{t'\neq t'}{}'\sum_{t'\neq t}{}'\frac{a(t|H|t')(t'|H|t'')(t''|H|t_0)}{\{E_0-(t''|H|t'')\}\{E_0-(t'|H|t')\}\{E_0-(t|H|t)\}}\,, \qquad (14)$$

and

$$a(t_0|H|t_0)+\sum_t \frac{a(t_0|H|t)(t|H|t_0)}{E_0-(t|H|t)}+\sum_{t\neq t'}{}'\frac{a(t_0|H|t)(t|H|t')(t'|H|t_0)}{\{E_0-(t|H|t)\}\{E_0-(t'|H|t')\}}$$
$$+\sum_{t\neq t'}{}'\sum_{t'\neq t''}{}'\frac{a(t_0|H|t)(t|H|t')(t'|H|t'')(t''|H|t_0)}{\{E_0-(t|H|t)\}\{E_0-(t'|H|t')\}\{E_0-(t''|H|t'')\}}=aW. \qquad (15)$$

These formulas will be contrasted with Kramers' formula although we have left P^σ as it is.

Further $(t|H|t)$ can always be divided into the term, $(t|H'|t)$, which relates to the spin permutations $P^\sigma(P^\sigma\neq E)$ and the term, E_t, which does not relate to P^σ and is principally considered to be the orbital energies and the Coulomb energies of the N electron system in the excited configuration ψ_t:

$$(t|H|t)=E_t+(t|H'|t). \qquad (16)$$

If it is allowed that E_0 is not concerned with the spin permutations P^σ and the exchange terms contained in $(t|H'|t)$ are smaller than E_t-E_0, the factors $\{E_0-(t|H|t)\}$ which appear in the denominators of Eq. (15) can be expanded as

$$\{E_0-(t|H|t)\}^{-1}=-\frac{1}{(E_t-E_0)}\left\{1-\frac{(t|H'|t)}{E_t-E_0}+\frac{(t|H'|t)^2}{(E_t-E_0)^2}-\cdots\right\}. \qquad (17)$$

The first assumption that $E_0=(t_0|H|t_0)$ is not concerned with $P^a(P^a\neq E)$ is equivalent to saying that all spin states of the ground configuration are degenerate, and it is not general, but the generalization to another case will be easily done.

Thus the expression (15) combined (17), can be rewritten as follows:

$$(t_0|H|t_0)-\sum_t \frac{(t_0|H|t)(t|H|t_0)}{E_t-E_0}$$

$$+\sum_t \frac{(t_0|H|t)(t|H'|t)(t|H|t_0)}{(E_t-E_0)^2}+\sum_{t\neq t'}\sum' \frac{(t_0|H|t')(t'|H|t)(t|H|t_0)}{(E_t-E_0)(E_{t'}-E_0)}$$

$$-\sum_t \frac{(t_0|H|t)(t|H'|t)^2(t|H|t_0)}{(E_t-E_0)^3}-\sum_{t\neq t'}\sum' \frac{2(t_0|H|t)(t|H'|t)(t|H|t')(t'|H|t_0)}{(E_t-E_0)^2(E_{t'}-E_0)}$$

$$-\sum_{t\neq t'\neq t''}\sum\sum \frac{(t_0|H|t)(t|H|t')(t'|H|t'')(t''|H|t_0)}{(E_t-E_0)(E_{t'}-E_0)(E_{t''}-E_0)}+\cdots=W. \qquad (18)$$

It will be expected from (18) that the degeneracy in the ground configuration is partly removed by the third-order or the fourth-order perturbation when all the exchange interactions are assumed to be perturbations. This expression (18) will be useful to the many electron problems in which the interaction between the orbital configurations of electrons must be considered and all exchange integrals, which are contained in $(t|H'|t)$ (and $(t_0|H|t_0)$) can be assumed to be considerably smaller than the differences, E_t-E_0 (that is, approximately the differences between the ground and the excited orbital energies of the jumped electron).

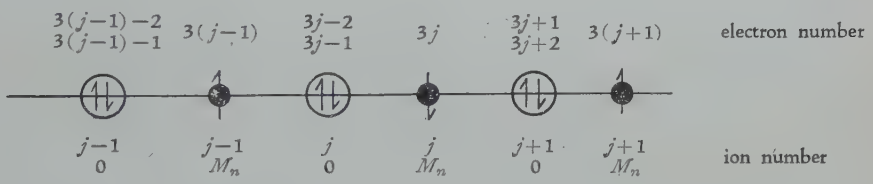


Fig. 1. Ground configuration of a linear lattice of MnO ($3N$ electron system)

§ 3. Superexchange interaction in a linear lattice

The superexchange interaction in a crystal, for example MnO, can be calculated by making use of the preceding formula. For the sake of simplicity we take the linear lattice, in which Mn ions and O ions are arranged alternatively as shown in Fig. 1, without loss of generality owing to the axial symmetry of the p–orbit in the negative ions, and in the ground state of this system we take only one electron on a Mn ion and two electrons on an O ion. The two electrons on a negative ion stay in the identical p–orbit actually, but for the present we regard the two orbits as distinct and those are denoted by p and p'.

The ground configuration of this model, the $3N$ electron system, can be represented by the function,

$$\psi_0=\prod_{j=1}^{N} p_j(3j-2)p_j'(3j-1)d_j(3j), \tag{19}$$

where $p_j(3j-2)$ is the orbital wave function of the $(3j-2)$th electron in the p–orbit of the jth O ion and $d_j(3j)$ is the orbital wave function of the $3j$th electron in the $3d$–orbit of the jth Mn ion. The same can be said of $p_j'(3j-1)$.

As to the excited configurations we take into account only the configurations that an electron has jumped from an O ion into a certain orbit of the adjacent Mn ions. That orbit may be already occupied by one electron or unoccupied and the wave function of the orbit will be denoted by s including both cases. It will be easily seen from Fig. 1 that an electron on the tth O ion can be translated to the right-hand Mn ion t or to the left-hand Mn ion $t-1$, and these excited configurations are shown by

$$\psi_{\overrightarrow{t}}=\prod_{\substack{j=1\\ \neq t}}^{N} p_j(3j-2)p_j'(3j-1)d_j(3j)p_t(3t-2)s_t(3t-1)d_t(3t), \tag{20, 1}$$

and

$$\psi_{\overleftarrow{t}}=\prod_{\substack{j=1\\ \neq t}}^{N} p_j(3j-2)p_j'(3j-1)d_j(3j)s_{t-1}(3t-2)p_t'(3t-1)d_t(3t). \tag{20, 2}$$

As two wave functions of p–state in an O ion, p and p', are regarded to be independent or orthogonal with each other, the following excited configurations in which the electrons $3j-1$ and $3j-2$ are interchanged in the expressions (20) must be simultaneously considered :

$$\psi'_{\overrightarrow{t}}=\prod_{\substack{j=1\\ \neq t}}^{N} p_j(3j-2)p_j'(3j-1)d_j(3j)p_t'(3t-1)s_t(3t-2)d_t(3t), \tag{21, 1}$$

and

$$\psi'_{\overleftarrow{t}}=\prod_{\substack{j=1\\ \neq t}}^{N} p_j(3j-2)p_j'(3j-1)d_j(3j)s_{t-1}(3t-1)p_t(3t-2)d_t(3t). \tag{21, 2}$$

Letting aside all the permutations except the interchanges between the electrons which are the nearest neighbours with each other, the matrix elements (13) with the wave functions (19), (20) and (21) can be simply written down owing to the orthogonality relations among the orbital wave functions p, p', d, and s. First we have

$$\begin{aligned}(t_0|H|t_0)=E_0'+\sum_{j=1}^{N}[&J_{pp'}P_{3j-2,\,3j-1}+J_{pd}(P_{3j-2,\,3j}+P_{3j+1,\,3j})\\ &+J_{p'd}(P_{3j+2,\,3j}+P_{3j-1,\,3j})+J_{dd}P_{3j,\,3(j+1)}],\end{aligned} \tag{22}$$

where E_0' is a sum of the orbital energies and the Coulomb energies of the $3N$ electron system which are not concerned with the electron interchanges and J_{pd} is the exchange integral between the p–orbit on an O ion and the d–orbit on the adjacent Mn ion, etc. By hypothesis there is no exchange interaction between two Mn ions so that $J_{dd}=0$ will be held. And $P_{i,j}$ indicates the operator which interchanges the spin co-ordinates of electrons i and j.

Usually these interchange operators are expressed by spin operators as

$$P_{i,j}=-\frac{1}{2}(1+4\boldsymbol{s}_i\cdot\boldsymbol{s}_j). \tag{23}$$

As stated above, two electrons on an O ion will be actually regarded to be in a single orbit having antiparallel spins, the restrictions

$$\boldsymbol{s}_{3j-2}+\boldsymbol{s}_{3j-1}=0\,,\quad (j=1,\,2,\,\cdots N), \tag{24}$$

will be imposed on the formula (22), and using the relations:

$$P_{3j-2,\,3j-1}=1,\quad \text{and}\quad P_{3j\pm2,\,3j}+P_{3j\pm1,\,3j}=-1, \tag{25}$$

the expression (22) is reduced to the constant which is denoted by E_0:

$$(t_0|H|t_0)=E_0'-2NJ_{pd}=E_0\,, \tag{26}$$

where $J_{pp'}$ $(p=p')$ is eliminated, for J_{pp} is no more an exchange integral but a Coulomb integral and should be included in E_0'.

$(t_0|H|t)$ and $(t|H|t_0)$ in Eqs. (13) are the factors which are connected with the transition of an electron and are reduced to

$$(t_0|H|\vec{t})=b+b'P_{3t-1,\,3t}\,, \tag{27, 1}$$

where

$$b=\int p_t^*(3t-1)Hs_t(3t-1)\,d\tau_{3t-1}\,,$$

$$b'=\int p_t^*(3t-1)\,d_t^*(3t)Hd_t(3t-1)\,s_t(3t)\,d\tau_{3t-1}\,d\tau_{3t}\,.$$

The first term of the right-hand side of $(27\cdot1)$ corresponds to the direct transition, $p_t\rightarrow s_t$, and the second term corresponds to the indirect transition, $p_t\rightarrow d_t$, $d_t\rightarrow s_t$, which is supposed to be most probable in indirect transitions. Similarly from $\psi_{\overleftarrow{t}}$, $\psi'_{\vec{t}}$ and $\psi'_{\overleftarrow{t}}$,

$$(t_0|H|\overleftarrow{t})=b+b'P_{3t-2,\,3(t-1)}\,, \tag{27, 2}$$

$$(t_0|H|\vec{t})'=b+b'P_{3t-2,\,3t}\,, \tag{27, 3}$$

and

$$(t_0|H|\overleftarrow{t})'=b+b'P_{3t-1,\,3(t-1)}\,. \tag{27, 4}$$

$(\vec{t}|H|t_0)$, etc., are also written by the complex conjugates of b and b'. As the indirect transition term, b' is estimated to be considerably smaller than the direct transition term, b, the indirect transition will be neglected in the later calculation.

At least two orbits are different in the excited configurations t and t' so that the integrals which are involved in $(t|H|t')$, Eqs. (13), will be certainly negligible in comparison with the exchange integrals, J_{pd}, etc. Then in the formula (18) we ignore the terms which contain the factor, $(t|H|t')$, namely a coupling between excited configurations. If, however, one needs to get the higher approximation the above-mentioned indirect transition and the coupling between excited configurations must be simultaneously taken into consideration. Thus because of our simplifications the important terms which are concerned with the spin operators in the formula (18) up to the fourth-order perturbation are the first term of the third-order perturbation:

$$\sum_t\frac{(t_0|H|t)\,(t|H'|t)\,(t|H|t_0)}{(E_t-E_0)^2}\,, \tag{28}$$

and the first term of the fourth-order perturbation :

$$-\sum_{t}\frac{(t_0|H|t)(t|H'|\vec{t})^2(\vec{t}|H|t_0)}{(E_t-E_0)^3}. \tag{29}$$

Now $(\vec{t}|H|\vec{t})$ can be written as follows :

$$\begin{aligned}(\vec{t}|H|\vec{t}) = E_1' &+ \sum_{\substack{j=1\\ \neq t}}^{N} J_{pp'} P_{3j-2,\,3j-1} + \sum_{\substack{j=1\\ \neq t-1}}^{N} J_{pd}(P_{3j+2,\,3j}+P_{3j+1,\,3j}) \\ &+ \sum_{\substack{j=1\\ \neq t}}^{N} J_{pd}(P_{3j-2,\,3j}+P_{3j-1,\,3j}) + J_{ps}P_{3t-2,\,3t-1} + J_{sd}P_{3t-1,\,3t} \\ &+ J_{pd}(P_{3t-2,\,3(t-1)}+P_{3t-2,\,3t}) + J_{ps}(P_{3t+1,\,3t-1}+P_{3t+2,\,3t-1}),\end{aligned} \tag{30}$$

where E_1' is the constant which contains the orbital energies and the coulomb energies in the excited configuration $\vec{t}$ and does not depend upon t. If we confine our consideration in the case where the excited orbit to which an electron on an O ion has been translated is an empty orbit we may impose only the restriction (24) upon the expression (30) and we have

$$(\vec{t}|H|\vec{t}) = E_1 - 2J_{pd}\boldsymbol{s}_{3t-2}\cdot\boldsymbol{s}_{3(t-1)} - 2(J_{sd}-J_{pd})\boldsymbol{s}_{3t-1}\cdot\boldsymbol{s}_{3t}, \tag{31, 1}$$

where

$$E_1 = E_1' - (2N-1)J_{pd} - \frac{1}{2}J_{sd}.$$

Similarly we obtain

$$(\overleftarrow{t}|H|\overleftarrow{t}) = E_1 - 2J_{pd}\boldsymbol{s}_{3t-1}\cdot\boldsymbol{s}_{3t} - 2(J_{sd}-J_{pd})\boldsymbol{s}_{3t-2}\cdot\boldsymbol{s}_{3(t-1)}, \tag{31, 2}$$

and using the functions (21·1) and (21·2)

$$(\vec{t}|H|\vec{t})' = E_1 - 2J_{pd}\boldsymbol{s}_{3t-1}\cdot\boldsymbol{s}_{3(t-1)} - 2(J_{sd}-J_{pd})\boldsymbol{s}_{3t-2}\cdot\boldsymbol{s}_{3t}, \tag{31, 3}$$

and

$$(\overleftarrow{t}|H|\overleftarrow{t})' = E_1 - 2J_{pd}\boldsymbol{s}_{3t-2}\cdot\boldsymbol{s}_{3t} - 2(J_{sd}-J_{pd})\boldsymbol{s}_{3t-1}\cdot\boldsymbol{s}_{3(t-1)}. \tag{31, 4}$$

Regarding the terms which are concerned with the spin operators as perturbations and putting $E_t = E_1$ and $(\vec{t}|H'|\vec{t}) = -2J_{pd}\boldsymbol{s}_{3t-2}\cdot\boldsymbol{s}_{3(t-1)} - 2(J_{sd}-J_{pd})\boldsymbol{s}_{3t-1}\cdot\boldsymbol{s}_{3t}$ etc., the third-order perturbing term (28) is written as follows :

$$\begin{aligned}\sum_{t}\frac{(t_0|H|t)(t|H'|t)(t|H|t_0)}{(E_t-E_0)^2} = -\frac{2b^2J_{sd}}{(E_1-E_0)^2}\sum_{t=1}^{N}&(\boldsymbol{s}_{3t-1}\cdot\boldsymbol{s}_{3t}+\boldsymbol{s}_{3t-2}\cdot\boldsymbol{s}_{3(t-1)} \\ &+\boldsymbol{s}_{3t-2}\cdot\boldsymbol{s}_{3t}+\boldsymbol{s}_{3t-1}\cdot\boldsymbol{s}_{3(t-1)}),\end{aligned} \tag{32}$$

where the sum over all excited configurations, $\vec{t}$, $\overleftarrow{t}$, $\vec{t}'$, and $\overleftarrow{t}'$ is taken. The right-hand side of this formula is reduced to zero owing to the restrictions of the zero spin in O ions, (24).

Therefore the spin-coupling between the magnetic ions does not present itself up to the third-order perturbation when the inner- and the inter-atomic exchange integrals are regarded as perturbations in comparison with the orbital splitting energy ($\approx E_1-E_0$). Then we should calculate the fourth-order term (29) from Eqs. (31) making use of the relation :

$$(\boldsymbol{s}_k\cdot\boldsymbol{s}_i)(\boldsymbol{s}_k\cdot\boldsymbol{s}_j)=\frac{1}{4}(\boldsymbol{s}_i\cdot\boldsymbol{s}_j)+\frac{i}{2}\boldsymbol{s}_k\cdot(\boldsymbol{s}_i\times\boldsymbol{s}_j).$$

We obtain from Eqs. (31),

$$\sum_t(t|H'|t)^2=3N(J_{pd}^2+(J_{sd}-J_{pd})^2)-8\sum_{t=1}^{N}J_{pd}(J_{sd}-J_{pd})\boldsymbol{s}_{3t}\cdot\boldsymbol{s}_{3(t-1)}\,,$$

and except the constant term the fourth-order term is given by

$$-\sum_t\frac{(t_0|H|t)(t|H'|t)^2(t|H|t_0)}{(E_t-E_0)^3}=\frac{8b^2J_{pd}(J_{sd}-J_{pd})}{(E_1-E_0)^3}\sum_{t=1}^{N}\boldsymbol{s}_{3t}\cdot\boldsymbol{s}_{3(t-1)}\,. \qquad (33)$$

The last formula shows the spin-coupling between the electrons on Mn ions and has the same form as the ordinary exchange interaction. The effective exchange integral, $-8b^2J_{pd}(J_{sd}-J_{pd})/(E_1-E_0)^3$, has a positive sign as long as $J_{pd}<0$ and $J_{sd}>0$ which will be in accord with the Hund rule and it gives a ferromagnetic interaction. On the other hand the effective exchange integral becomes ferromagnetic having no relation to the signs of J_{sd} and J_{pd} if the absolute value of J_{sd} should be smaller than the absolute value of J_{pd}. It should be noted, however, that these conclusions are derived only if the orbits d and s of the same Mn ion are independent. The same result will also be obtained from the four-electron system making use of Serber's method in the Appendix.

The generalization of our calculation to the case in which the magnetic ions have more than one $3d$ electron can be easily made and a result quite similar to (33) is obtained except that the spin operator of the single electron is replaced by the total spin operator of the magnetic ion.

§ 4. Antiferromagnetic coupling in the superexchange interaction

In a real compound the preceding discussion is not necessarily sufficient to decide whether the superexchange interaction is ferro- or antiferro-magnetic, because the excited configuration in which an electron on a negative ion has jumped into the level of the adjacent magnetic ion which is already occupied by an electron should be reasonably included in the previous calculations. This excited configuration becomes more important when the splitting caused in $3d$ levels of magnetic ions by the surrounding crystal field is appreciable and the inner exchange integral in a magnetic ion is not so great. In practice the level splitting will not be expected to be greater than the inner exchange integral.

When the electron on a negative ion goes to the level which is already occupied by another electron, the additional restriction on the spins in the excited configuration $\vec{t}$,

$$\boldsymbol{s}_{2t-1}+\boldsymbol{s}_{3t}=0\,, \qquad (34)$$

must be required because of the exclusion principle.

By use of Eqs. (24) and (34) the expression (31·2) is further reduced to

$$(\vec{t}|H|\vec{t})=E_a-2J_{pd}\boldsymbol{s}_{3t}\cdot\boldsymbol{s}_{3(t-1)}\,, \qquad (35)$$

where

$$E_a = E_1' - \left(2N + \frac{1}{2}\right) J_{pd} .$$

J_{sd} is no more an exchange integral but a coulomb integral and is eliminated from E_a for it should be already counted in E_1'. Strictly speaking the present E_1' is different from the previous E_1' in Eq. (30), but the difference will be small. $(\overleftarrow{t}|H|\overleftarrow{t})$, $(\overrightarrow{t}|H|\overrightarrow{t})'$ and $(\overleftarrow{t}|H|\overleftarrow{t})'$ are similarly rewritten. Then the first important term of the spin-coupling is derived from the third-order perturbation, the formula (28), and newly putting

$$E_t = E_a \quad \text{and} \quad (\overrightarrow{t}|H'|\overrightarrow{t}) = -2J_{pd}\boldsymbol{s}_{2t}\cdot\boldsymbol{s}_{3(t-1)} , \quad \text{etc.},$$

it becomes

$$\sum_t \frac{(t_0|H|t)(t|H'|t)(t|H|t_0)}{(E_t - E_0)^2} = -\frac{8b^2 J_{pd}}{(E_a - E_0)^2} \sum_{t=1}^{N} \boldsymbol{s}_{2t}\cdot\boldsymbol{s}_{3(t-1)} . \qquad (36)$$

The above spin-coupling makes an antiferromagnetic coupling because its effective exchange integral $8b^2 J_{pd}/(E_a - E_0)^2$ is negative if $J_{pd} < 0$ as in Section 3.

This antiferromagnetic spin-coupling is the third-order and will give a greater contribution to the superexchange interaction than the fourth-order ferromagnetic spin-coupling in the previous section, although the energy differences in the denominators of the effective exchange integrals are different. This difference will be neglected if the exchange integrals, J_{pd} and J_{sd}, are small compared with the excitation energy which is necessary for the electron to jump from a negative ion to the adjacent magnetic ion.

The generalization of our method to the case of several electrons in a magnetic ion instead of one electron can be achieved with the slight modification in which the excited configurations that an electron has jumped from a negative ion to each singly-occupied orbit of a magnetic ion will be simultaneously compounded, and assuming that the orbital energy splitting in $3d$-shells is not so large, we can obtain the same expression of the superexchange interaction in terms of the resultant spin vectors of magnetic ions.

In either compound which contains the magnetic ions with more or less than half-filled $3d$-shells the third-order antiferromagnetic spin-coupling will be more important generally. In the former case the excited state to which an electron on a negative ion has been translated is either $4s$ level or $3d$ level and the $3d$ level is to be occupied by an electron. The ferromagnetic interaction caused from the first excited configuration with the $4s$ level will be weak when the orbital energy splitting between $4s$ and $3d$ levels has occurred to some extent and the antiferromagnetic interaction will overwhelm the other. Then in a compound with the magnetic ions which possess more than 5 electrons in the $3d$ shells, an antiferromagnetism is likely to take place as Anderson concluded, and these conclusions do not contradict with the experimental facts at all.

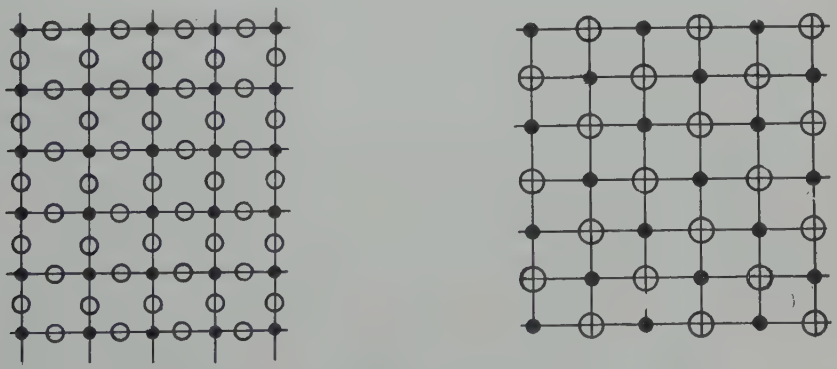
On the other hand in the case of magnetic ions with less than half-filled $3d$ shells a ferromagnetic spin-coupling can be seen even when the excited state to which an electron jumps from a negative ion is $3d$ state, but it seems that the antiferromagnetic coupling which must be naturally taken into account even in this case is superior to the ferromagnetic coupling as mentioned before. From the fact that this does not hold in CrTe

which shows a ferromagnetism it will have to hold that $E_a \gg E_1$ or $J_{sl}-J_{pl}$ has a considerable magnitude in order that the absolute value of the effective exchange integral $-8b^2J_{pl}(J_{sl}-J_{pl})/(E_1-E_0)^3$ is greater than the absolute value of $8b^2J_{pl}/(E_a-E_0)$, or else it will be attributable to another interaction, for example, the direct exchange interaction. It will be apt to satisfy the first condition, but if J_{sl} is larger than the orbital excitation energy of the jumped electron, E_1-E_0 becomes small or negative and our calculations of the superexchange interaction will be unwarranted. Then another method to calculate the ferromagnetic superexchange interaction, for example, the method shown in the Appendix, will be necessary.

§ 5. Conclusion

From our calculations we are inclined to believe that the magnetism of any compound in which the direct exchange interaction does not play an important part of the magnetic interaction is essentially antiferromagnetic. CrTe is an exceptional case where a more detailed calculation is required. The best example of our criterion will be CrO, but unfortunately it is not yet found in nature. Nevertheless manganites, e. g. $LaMnO_3$, etc., which have been recently studied by Jonker and van Santen will be suitable as test examples, for these materials have the perovskite crystal structure and the nearest neighbour-interaction between Mn ions is the superexchange interaction. $Ca^{2+}Mn^{4+}O_3$, $Sr^{2+}Mn^{4+}O_3$ and $Ba^{2+}Mn^{4+}O_3$ are probably antiferromagnetic and these facts support our conclusions as well as the facts that CrS, CrSb, Cr_2O_3 and MnO_2 are antiferromagnetic compounds. $La^{3+}Mn^{3+}O_3$ is not yet ascertained whether it is ferro- or antiferro-magnetic, but in either case the Curie temperature will be considerably low.

The linear lattice model has been used in our calculations, but it is easily seen that the three-dimensional cubic lattices are constructed by the superposition of the linear lattices as shown in Fig. 2 (a) and (b). The one (a) corresponds to $LaMnO_3$, etc., and the other (b) corresponds to MnO, etc., which has four sets of the simple cubic antiferromagnetic sublattice (a).



(a) (b)

Fig. 2. Two-dimensional square lattices instead of three-dimensional

On the other hand the impurity semiconducting magnetic compounds, that is, ferrites, mixed manganites, etc., exhibit mostly ferromagnetic properties and these facts are explained by Néel's theory of uncompensated antiferromagnetism or ferromagnetism,[2] but in exceptional cases the experimental values of the saturation magnetizations of the mixed manganites[7] cannot be consistent with the concepts of the uncompensated antiferromagnetism. In this case the interaction between the Mn ions with different ionic valencies has been thought to make the magnetic moments strongly parallel and Zener[11] attributed the interaction to the double exchange interaction. Perhaps a certain interaction between Mn^{3+} and Mn^{4+} ions will be considered to overwhelm the above-mentioned superexchange interaction which is assumed to be antiferromagnetic in this material and the ferromagnetism will take place in the mixed manganites. This sort of interaction between the magnetic ions which have different ionic valencies and are intermediated with each other by non-magnetic negative ions will be discussed in another paper.

In conclusion, the writer wishes to express his cordial thanks to Professor K. Ariyama and Dr. S. Nakajima for their interest in this work and their invaluable advice.

Appendix

We take the local model of a magnetic compound, two magnetic ions possessing one electron and one negative ion with two electrons in the middle of two magnetic ions, namely a 4-electron system such as Anderson used, and we shall seek the value of the energies of the spin states of this 4-electron system by means of Serber's method,[6] making use of the irreducible representation of the symmetric permutation group.

Generally the 4-electron system has the spin states of two singlets, three triplets and one quintet, but as the two electrons on a negative ion are assumed to be on the same orbit, these spin states should be reduced and the quintet is entirely omitted. In the ground configuration the permutation matrices will be limited in the reduced representation in which the interchange of two electrons on a negative ion is in identity when taking a diagonal representation of this interchange. Thus the four-electron problem is actually reduced to a two-electron problem and we have one singlet and one triplet, which are assumed to be degenerate, in the ground configuration.

As mentioned in the text the ground configuration in which two electrons are on a negative ion and the other two are on two magnetic ions respectively is combined with the excited configurations in which an electron on a negative ion has been translated to the left- or the right-hand magnetic ion. We use the same notation as in the text and construct the energy matrices for the singlet state and the triplet state as follows. The ground configuration can be expressed by the function :

$$\psi_g = p(1)p(2)d_1(3)d_2(4),$$

and two excited configurations in which an electron has jumped from a negative ion to the right- and the left-hand magnetic ions are respectively expressed by

$$\psi_p = p(1)s_1(2)d_1(3)d_2(4),$$

and

$$\psi_l = p(1)s_2(2)d_1(3)d_2(4).$$

Assuming that all orbital wave functions are orthogonal with each other and there is no overlap between two d- or s-wave functions, we can obtain the following secular equations from the permutation matrices:[6] for the triplet state $S=1$,

$$\begin{vmatrix} 2A & 0 & 0 & 2b & 0 & 0 & 2b \\ 0 & B_{11} & B_{12} & B_{13} & -E_2 & 0 & 0 \\ 0 & B_{12} & B_{22} & B_{23} & 0 & -E_2 & 0 \\ 2b & B_{13} & B_{23} & B_{33} & 0 & 0 & E_2 \\ 0 & -E_2 & 0 & 0 & B_{11} & -B_{12} & B_{13} \\ 0 & 0 & -E_2 & 0 & -B_{12} & B_{22} & -B_{23} \\ 2b & 0 & 0 & E_2 & B_{13} & -B_{23} & B_{33} \end{vmatrix} = 0,$$

$$A = E_0 - 2J_{pd} - W,$$

$$B_{11} = E_1 - J_{ps} - W, \qquad B_{12} = -\frac{1}{\sqrt{2}} J_{sd},$$

$$B_{22} = E_1 - J_{ps} - J_{pd} - \frac{1}{2} J_{sd} - W, \qquad B_{23} = \frac{1}{\sqrt{2}} (2J_{pd} - J_{sd}),$$

$$B_{33} = E_1 + J_{ps} - J_{pd} - \frac{1}{2} J_{sd} - W, \qquad B_{13} = \frac{1}{2} J_{sd},$$

and for the singlet state $S=0$,

$$\begin{vmatrix} 2A & 0 & 2b & 0 & 2b \\ 0 & C_{11} & C_{12} & -E_2 & 0 \\ 2b & C_{12} & C_{22} & 0 & E_2 \\ 0 & -E_2 & 0 & C_{11} & -C_{12} \\ 2b & 0 & E_2 & -C_{12} & C_{22} \end{vmatrix} = 0,$$

$$C_{11} = E_1 - J_{ps} + J_{pd} + \frac{1}{2} J_{sd} - W,$$

$$C_{22} = E_1 + J_{ps} - J_{pd} - \frac{1}{2} J_{sd} - W,$$

$$C_{12} = -\frac{\sqrt{3}}{2} J_{sd},$$

where E_0 and E_1 are sums of the orbital and the coulomb energies in the ground- and the excited-configurations respectively. E_2 is the resonance energy between two excited configurations and is expressed by

$$E_2 = \iint p^*(2)s_1^*(1) \frac{e^2}{r_{12}} p(1)s_2(2)d\tau_1 d\tau_2.$$

It is noted that the exchange integral J_{ps} comes out in these determinants because of the local model of a crystal compound, but it is not concerned with the final result. These determinants can be divided into the part which does not combine with the ground state and the part which combines with that. The latter parts for $S=1$ and $S=0$ are

$$\begin{vmatrix} A & 0 & 0 & 2b \\ 0 & B_{11}-E_2 & B_{12} & B_{13} \\ 0 & B_{12} & B_{22}+E_2 & B_{23} \\ 2b & B_{13} & B_{23} & B_{33}+E_2 \end{vmatrix}=0, \quad \text{and} \quad \begin{vmatrix} A & 0 & 2b \\ 0 & C_{11}+E_2 & C_{12} \\ 2b & C_{12} & C_{22}+E_2 \end{vmatrix}=0.$$

We can solve these secular equations exactly, but in order to compare the solutions with the previous results in the text (formula (33)) we shall solve these equations by means of perturbations and obtain the energy difference between the singlet and the triplet as follows:

$$W_1-W_3=-\frac{8b^2}{(E_1-E_0)^3}J_{pd}(J_{sd}-J_{pd}).$$

This result coincides exactly with the previous result (33) and the resonance energy E_2 between the excited configurations does not appear up to the fourth-order perturbation. And this warrants our approximation taken in Section 3.

References

1) C. G. Shull and J. S. Smart, Phys. Rev. **76** (1949), 1256; C. G. Shull, W. A. Strauser and E. O. Wollan, Phys. Rev. **83** (1951), 333.
2) L. Néel, Ann. Physique **3** (1948), 137.
3) J. H. Van Vleck, Journ. phys. et radium **12** (1951), 262.
4) P. W. Anderson, Phys. Rev. **79** (1950), 351.
5) H. A. Kramers, Physica **1** (1934), 182.
6) R. Serber, Phys. Rev. **45** (1934), 461; J. Chem. Phys. **2** (1934), 697.
7) G. H. Jonker and J. H. van Santen, Physica **16** (1950), 337.
8) K. Honda and T. Sone, Sci, Rep. Tohoku Imp. Univ. **3** (1914), 223; G. Foëx and M. Graff, Comptes Rendus **209** (1939), 160.
9) A. I. Snow, Phys. Rev. **85** (1952), 365; R. A. Erickson, Phys. Rev. **85** (1952), 745.
10) See reference 3 above, p. 274.
11) C. Zener, Phys. Rev. **82** (1951), 403

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On the β-Ray Angular Correlations

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The angular distribution functions of β-rays that are used to obtain the angular correlation functions are calculated taking into account the effect of the nuclear charge. The calculations are performed up to the second forbidden transitions for each β-decay interaction type of the Fermi theory separately but including the mixture of the nuclear matrix elements. To obtain the angular correlation functions easily in the case of the mixed nuclear matrix elements they are given in considerably simple forms in two interesting cases. Also in the appendix, transformation coefficients $(j_1 3 m_1 m_2 | j_1 3 j m)$ are given.

§ 1. Introduction

When two particles are emitted successively from a nucleus, there is angular correlation between them.[1] This evidence is now well known. Studies of the angular correlation is useful for understanding spins and parities of nuclei. Besides them, when β-decays are concerned, it can be used to decide the β-decay interaction type.

Many theories have been issued concerning the angular correlation. These theories are divided into two, the one is that which is common to all kinds of radiations and the other is the study of special cases. The first was investigated by Falkoff and Uhlenbeck,[2] Racah,[3] and Lloyd.[4] As to the latter, there are studies by Hamilton,[1)5)] Goertzel,[6] Ling Jr. and Falkoff,[2] Lloyd[8] and others for $\gamma-\gamma$, and for the cases internal conversions are included, there are detailed calculations by Rose *et al.*[9]

For the cases β-rays are included, Falkoff and Uhlenbeck[10] and Fuchs and Lennox[11] studied, but they either omitted the effect of the nuclear charge[10] or took it into account only in the approximation of $\alpha Z \ll 1$.[11] Therefore, in this paper we calculate the angular distribution functions* of β-rays taking into account the effect of the nuclear charge perfectly.† ††

§ 2. General theory

In this section we introduce the forms of the angular correlation function $W(\theta)$

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* As to the meaning of angular distribution function see Section 2.

† But the effect of the finite nuclear size is not considered explicitly.

†† Recently the authors knew that Fuchs and Al-Ghita investigated this problem; M. Fuchs, Thesis, (University of Michigan, 1951); M. K. Al-Ghita, Thesis, (University of Michigan, 1951). But the authors have not seen them yet.

which are convenient in the cases of the mixed nuclear matrix elements. Mainly we follow the procedures of Falkoff and Uhlenbeck.[2]

We consider only the directions of particles, and do not observe the polarizations of them. Then the angular correlation function $\mathcal{W}(\theta)$, the relative probability that two particles are emitted with the angle θ, is[1]

$$\mathcal{W}(\theta)=\boldsymbol{S}_1\boldsymbol{S}_2\sum_{l,n}\Big|\sum_m(B_m|H_1(\boldsymbol{k}_1)|A_l)\,(C_n|H_2(\boldsymbol{k}_2)|B_m)\Big|^2. \tag{1}$$

The notation is as follows: the nucleus changes $A_l\to B_m\to C_n$, l, m and n are the z-components of the total angular momenta, $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ are the directions of the first and the second particles, and $\boldsymbol{S}_1$ and $\boldsymbol{S}_2$ indicate the sums over all the directional arguments (spin etc.) except for $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$. Generally, in the right-hand side of Eq. (1) there are interferences between different m's; but when we select the z-axis as $\boldsymbol{k}_1$, the interferences vanish[13] and Eq. (1) becomes

$$\mathcal{W}(\theta)=\sum_m\Big[\sum_l\{\boldsymbol{S}_1|(B_m|H_1(0)|A_l)|^2\}\sum_n\{\boldsymbol{S}_2|(C_n|H_2(\theta)|B_m)|^2\}\Big]. \tag{2}$$

We put

$$\boldsymbol{S}_1|(B_m|H_1(\theta)|A_l)|^2\equiv p_{lm}(\theta),\quad \boldsymbol{S}_2|(C_n|H_2(\theta)|B_m)|^2\equiv P_{mn}(\theta). \tag{3}$$

$p_{lm}(\theta)$ is the relative probability that the nucleus changes from A_l to B_m and the first particle is emitted into the direction θ, and $P_{mn}(\theta)$ is that of the second particle. Then Eq. (2) becomes

$$\mathcal{W}(\theta)=\sum_{l,m,n}p_{lm}(0)P_{mn}(\theta). \tag{4}$$

Let $T_{i_1,\cdots,i_L}$ be the irreducible tensors of the L-th rank for the rotations of 3-dimensional space. The interaction Hamiltonian is invariant under the space rotations, so that it can be represented as follows:

$$H=\sum_{T(\boldsymbol{X}_i)}a\,[T(\boldsymbol{X}_i)]\sum_{i_1,\cdots,i_L}T_{i_1,\cdots,i_L}(\boldsymbol{X}_i)\,T_{i_1,\cdots,i_L}(\boldsymbol{A}_i), \tag{5}$$

where $\boldsymbol{X}_i$ are vector operators for the nucleus, $\boldsymbol{A}_i$ are argument vectors for the emitted particle, $a\,[T(\boldsymbol{X}_i)]$ are numerical coefficients and $\sum_{T(\boldsymbol{X}_i)}$ denotes the sum over various irreducible tensors (including various L's). In the theory of the angular correlation, the magnetic quantum numbers play important parts, so that it is convenient to use the polarized solid harmonics[2] $\mathcal{Y}_{LM}$ normalized as follows:

$$\sum_{M=-L}^{L}\mathcal{Y}_{LM}(\boldsymbol{X}_i)\mathcal{Y}^*_{LM}(\boldsymbol{A}_i)\equiv\sum_{i_1,\cdots,i_L}T_{i_1,\cdots,i_L}(\boldsymbol{X}_i)\,T_{i_1,\cdots,i_L}(\boldsymbol{A}_i). \tag{6}$$

These polarized solid harmonics have the following properties. Let J, m and α be the total angular momentum, its z-component and other quantum numbers of the initial nucleus respectively, and J', m' and α' be those of the final nucleus, then

$$(\alpha'J'm'|\mathcal{Y}_{LM}(\boldsymbol{X}_i)|\alpha Jm)=\mathfrak{M}(\alpha,\alpha',J,J',\boldsymbol{X}_i)\,(JLmM|JLJ'm'), \tag{7}$$

where $\mathfrak{M}(\alpha,\alpha',J,J',\boldsymbol{X}_i)$ is a complex number independent of m and m', and is called

a reduced nuclear matrix element. $(JLmM|JL'J'm')$ are transformation coefficients for the vector addition,[14] and real numbers. They vanish unless $m+M=m'$, and this shows the selection rule for the magnetic quantum number.

From Eqs. (5) and (6)

$$H=\sum_{T(X_i)} a[T(X_i)]\sum_{M} \mathcal{Y}_{LM}(X_i)\mathcal{Y}^{*}_{LM}(A_i). \tag{8}$$

By Eqs. (7) and (8), Eq. (3) becomes

$$p_{mm'}(\theta)=S|\sum_{T(X_i)} a[T(X_i)]\,\mathfrak{M}(X_i)\,(JLmM|JLJ'm')\,\mathcal{Y}^{*}_{LM}(A_i)|^2 \tag{9}$$

with $m+M=m'$.

In the right-hand side of Eq. (9) the θ-dependent parts are $\mathcal{Y}^{*}_{LM}(A_i)$. Let $\sum_{T_L(X_i)}$ denote the sum over various irreducible tensors retaining the L constant, then Eq. (9) becomes

$$\begin{aligned} p_{mm'}(\theta)&=S|\sum_{L}\sum_{T_L(X_i)} a[T(X_i)]\,\mathfrak{M}(X_i)\,(JLmM|JLJ'm')\,\mathcal{Y}^{*}_{LM}(A_i)|^2 \\ &=\sum_{L}(JLmM|JLJ'm')^2 S|\sum_{T_L(X_i)} a[T(X_i)]\,\mathfrak{M}(X_i)\,\mathcal{Y}^{*}_{LM}(A_i)|^2 \\ &+\sum_{L_1<L_2}(JL_1mM|JL_1J'm')\,(JL_2mM|JL_2J'm')\,S\sum_{T_{L_1}(X_i)}\sum_{T_{L_2}(X_j)} \\ &\{a^*[T(X_i)]\,a[T(X_j)]\,\mathfrak{M}^*(X_i)\mathfrak{M}(X_j)\,\mathcal{Y}_{L_1M}(A_i)\,\mathcal{Y}^{*}_{L_2M}(A_j)+\text{c.c.}\} \end{aligned} \tag{10}$$

with $m+M=m'$.

We put

$$\begin{aligned} F_{LL}^{M}(\theta)&=S|\sum_{T_L(X_i)} a[T(X_i)]\,\mathfrak{M}(X_i)\,\mathcal{Y}^{*}_{LM}(A_i)|^2, \\ F_{L_1L_2}^{M}(\theta)&=S\sum_{T_{L_1}(X_i)}\sum_{T_{L_2}(X_j)}\{a^*[T(X_i)]\,a[T(X_j)]\,\mathfrak{M}^*(X_i)\mathfrak{M}(X_j) \\ &\quad\cdot\mathcal{Y}_{L_1M}(A_i)\,\mathcal{Y}^{*}_{L_2M}(A_j)+\text{c.c.}\}, \end{aligned} \tag{11}$$

then Eq. (10) becomes

$$p_{mm'}(\theta)=\sum_{L_1\le L_2}{}'(JL_1mM|JL_1J'm')\,(JL_2mM|JL_2J'm')\,F_{L_1L_2}^{M}(\theta) \tag{12}$$

with $m+M=m'$.

$F_{L_1L_2}^{M}(\theta)$ are called angular distribution functions. We obtain the angular correlation function by inserting Eq. (12) into Eq. (4).

In the formula (12) the transformation coefficients are determined entirely by the group-theoretical method, and the angular distribution functions $F_{L_1L_2}^{M}(\theta)$ are to be determined in each case. M takes the values from $-L_1$ to $L_1(L_1\le L_2)$. However, these $2L_1+1$ functions are not independent of each other, and if we know a suitable one among them, the others can be known mathematically. The reason is as follows. As $S\mathcal{Y}_{L_1M}\mathcal{Y}^{*}_{L_2M}$ is the only part that is connected with θ, we observe that part only.

$$\begin{aligned} S\mathcal{Y}_{L_1M}\mathcal{Y}^{*}_{L_2M}&=S(-1)^M\mathcal{Y}_{L_1M}\mathcal{Y}_{L_2-M} \\ &=S\sum_{J}(-1)^M(L_2L_1-MM|L_2L_1J0)\,\mathcal{Y}_{J0}. \end{aligned} \tag{13}$$

There are following relations :[4]

$$\begin{aligned} \boldsymbol{S}\mathcal{Y}_{J0} &= u_J Y_{J0}, \qquad J: \text{ even}, \\ &= 0, \qquad J: \text{ odd}, \end{aligned} \tag{14}$$

where u_J are independent of M, and Y_{J0} are the spherical harmonics. We put $J=2n$, (n : integer) then

$$\begin{aligned} \boldsymbol{S}\mathcal{Y}_{L_1M}\mathcal{Y}^{*}_{L_2M} &= \sum_n (-1)^M (L_2L_1-MM\,|\,L_2L_1\,2n\,0)\,u_{2n}Y_{2n\,0}\,, \\ & L_2-L_1 \leq 2n \leq L_2+L_1\,. \end{aligned} \tag{15}$$

From Eqs. (11) and (15) we obtain the following parametrization :

$$\begin{aligned} F^{M}_{L_1L_2}(\theta) &= \sum_n (-1)^M (L_2L_1-MM\,|\,L_2L_1\,2n\,0)\,b^{(2n)}_{L_1L_2}P_{2n}(\cos\theta), \\ & L_2-L_1 \leq 2n \leq L_2+L_1\,, \end{aligned} \tag{16}$$

where $b^{(2n)}_{L_1L_2}$ are parameters and $P_{2n}(\cos\theta)$ are the Legendre polynomials :

$$P_n(x) = 1/(2^n n\,!)\cdot(d/dx)^n\{(x^2-1)^n\}. \tag{17}$$

The first four of Eq. (17) (even n) are

$$\begin{aligned} &P_0(\cos\theta)=1, \quad P_2(\cos\theta)=(3/2)\cos^2\theta-(1/2), \\ &P_4(\cos\theta)=(35/8)\cos^4\theta-(15/4)\cos^2\theta+(3/8), \\ &P_6(\cos\theta)=(231/16)\cos^6\theta-(315/16)\cos^4\theta+(105/16)\cos^2\theta-(5/16). \end{aligned} \tag{18}$$

Therefore, the problem reduces to the determination of $b^{(2n)}_{L_1L_2}$.

We write Eq. (16) explicitly in several cases. We multiply $b^{(2n)}_{L_1L_2}$ by suitable numerical factors, and write $a^{(2n)}_{L_1L_2}$.

1) $L_1=1,\ L_2=1$

$$\begin{aligned} F^{\pm 1}_{11}(\theta) &= a^{(0)}_{11}+a^{(2)}_{11}P_2(\cos\theta), \\ F^{0}_{11}(\theta) &= a^{(0)}_{11}-2a^{(2)}_{11}P_2(\cos\theta). \end{aligned} \tag{19}$$

2) $L_1=1,\ L_2=2$

$$\begin{aligned} F^{1}_{12}(\theta) &= -F_{12}{}^{1}(\theta) = a^{(2)}_{12}P_2(\cos\theta), \\ F^{0}_{12}(\theta) &= 0. \end{aligned} \tag{20}$$

3) $L_1=2,\ L_2=2$

$$\begin{aligned} F^{\pm 2}_{22}(\theta) &= a^{0}_{22}+2a^{(2)}_{22}P_2(\cos\theta)+a^{(4)}_{22}P_4(\cos\theta), \\ F^{\pm 1}_{22}(\theta) &= a^{(0)}_{22}-a^{(2)}_{22}P_2(\cos\theta)-4a^{(4)}_{22}P_4(\cos\theta), \\ F^{0}_{22}(\theta) &= a^{(0)}_{22}-2a^{(2)}_{22}P_2(\cos\theta)+6a^{(4)}_{22}P_4(\cos\theta). \end{aligned} \tag{21}$$

4) $L_1=2,\ L_2=3$

$$F^{2}_{23}(\theta) = -F^{-2}_{23}(\theta) = 5a^{(2)}_{23}P_2(\cos\theta)+2a^{(4)}_{23}P_4(\cos\theta),$$

$$F_{23}^{1}(\theta)=-F_{23}^{-1}(\theta)=\sqrt{10}\,a_{23}^{(2)}P_2(\cos\theta)-\sqrt{10}\,a_{23}^{(4)}P_4(\cos\theta),$$
$$F_{23}^{0}(\theta)=0. \qquad (22)$$

5) $L_1=3,\ L_2=3$

$$F_{33}^{\pm3}(\theta)=a_{33}^{(0)}+5a_{33}^{(2)}P_2(\cos\theta)+3a_{33}^{(4)}P_4(\cos\theta)+a_{33}^{(6)}P_6(\cos\theta),$$
$$F_{33}^{\pm2}(\theta)=a_{33}^{(0)}\qquad -7a_{33}^{(4)}P_4(\cos\theta)-6a_{33}^{(6)}P_6(\cos\theta),$$
$$F_{33}^{\pm1}(\theta)=a_{33}^{(0)}-3a_{33}^{(2)}P_2(\cos\theta)+a_{33}^{(4)}P_4(\cos\theta)+15a_{33}^{(6)}P_6(\cos\theta),$$
$$F_{33}^{0}(\theta)=a_{33}^{(0)}-4a_{33}^{(2)}P_2(\cos\theta)+6a_{33}^{(4)}P_4(\cos\theta)-20a_{33}^{(6)}P_6(\cos\theta). \qquad (23)$$

The angular distribution functions of γ-rays are given in reference 7 for the dipole and the quadrupole radiations.

$$F_{11}^{0}(\theta)=2|\alpha|^2\{1-P_2(\cos\theta)\},$$
$$F_{22}^{0}(\theta)=2|\beta|^2\{1+(5/7)P_2(\cos\theta)-(12/7)P_4(\cos\theta)\},$$
$$F_{12}^{1}(\theta)=2\sqrt{15}\,\mathcal{R}e(\alpha\beta^*)P_2(\cos\theta). \qquad (24)$$

α and β are the reduced nuclear matrix elements of the dipole and the quadrupole radiations respectively.

We obtain the angular correlation function $\mathcal{W}(\theta)$ from $F_{L_1L_2}^{M}(\theta)$ above shown, and Eqs. (12) and (4). In this case the sums of the products of the transformation coefficients appear. There are several relations between these sums. Falkoff and Uhlenbeck[2] calculated these relations in some cases. By the same method we obtain them in other cases.

Let the spin changes of the nucleus be $j-\Delta j\to j\to j+\Delta J$. For simplicity we put

$$g_{ii}^{m}=(j-\Delta j,i,m,0|j-\Delta j,i,j,m)^2,$$
$$d_{ii}^{m}=(j-\Delta j,i,m-1,1|j-\Delta j,i,j,m)^2+(j-\Delta j,i,m+1,-1|j-\Delta j,i,j,m)^2,$$
$$e_{ii}^{m}=(j-\Delta j,i,m-2,2|j-\Delta j,i,j,m)^2+(j-\Delta j,i,m+2,-2|j-\Delta j,i,j,m)^2,$$
$$f_{ii}^{m}=(j-\Delta j,i,m-3,3|j-\Delta j,i,j,m)^2+(j-\Delta j,i,m+3,-3|j-\Delta j,i,j,m)^2,$$
$$d_{i\,i+1}^{m}=(j-\Delta j,i,m-1,1|j-\Delta j,i,j,m)(j-\Delta j,i+1,m-1,1|j-\Delta j,i+1,j,m)$$
$$-(j-\Delta j,i,m+1,-1|j-\Delta j,i,j,m)$$
$$\times(j-\Delta j,i+1,m+1,-1|j-\Delta j,i+1,j,m),$$
$$e_{i\,i+1}^{m}=(j-\Delta j,i,m-2,2|j-\Delta j,i,j,m)(j-\Delta j,i+1,m-2,2|j-\Delta j,i+1,j,m)$$
$$-(j-\Delta j,i,m+2,-2|j-\Delta j,i,j,m)(j-\Delta j,i+1,m+2,-2|j-\Delta j,i+1,j,m),$$
$$G_{ii}^{m}=(j,i,m,0|j,i,j+\Delta J,m)^2,$$
$$D_{ii}^{m}=(j,i,m,1|j,i,j+\Delta J,m+1)^2+(j,i,m,-1|j,i,j+\Delta J,m-1)^2,$$
$$E_{ii}^{m}=(j,i,m,2|j,i,j+\Delta J,m+2)^2+(j,i,m,-2|j,i,j+\Delta J,m-2)^2,$$
$$D_{i\,i+1}^{m}=(j,i,m,1|j,i,j+\Delta J,m+1)(j,i+1,m,1|j,i+1,j+\Delta J,m+1)$$

$$-(j,i,m,-1|\,j,i,j+\Delta J,m-1)(j,i+1,m,-1|\,j,i+1,j+\Delta J,m-1). \tag{25}$$

We attach $'$ to the second transition.

When the first transition involves $L=1$ and 2, and the second transition involves $L=1$ and 2, $\mathcal{W}(\theta)$ is

$$\mathcal{W}(\theta)=\sum_m [g_{11}^m F_{11}^0(0)+d_{11}^m F_{11}^{\pm1}(0)+g_{22}^m F_{22}^0(0)+d_{22}^m F_{22}^{\pm1}(0)+e_{22}^m F_{22}^{\pm2}(0)+d_{12}^m F_{12}^1(0)]$$
$$\cdot[G_{11}^m F_{11}^{\prime 0}(\theta)+D_{11}^m F_{11}^{\prime\pm1}(\theta)+G_{22}^m F_{22}^{\prime 0}(\theta)+D_{22}^m F_{22}^{\prime\pm1}(\theta)+E_{22}^m F_{22}^{\prime\pm2}(\theta)+D_{12}^m F_{12}^{\prime 1}(\theta)]. \tag{26}$$

When we take the z-axis as the direction of the second particle and the θ-direction as that of the first particle, we obtain the same angular correlation function:

$$\mathcal{W}(\theta)=\sum_m [g_{11}^m F_{11}^0(\theta)+d_{11}^m F_{11}^{\pm1}(\theta)+g_{22}^m F_{22}^0(\theta)+d_{22}^m F_{22}^{\pm1}(\theta)+e_{22}^m F_{22}^{\pm2}(\theta)+d_{12}^m F_{12}^1(\theta)]$$
$$\cdot[G_{11}^m F_{11}^{\prime 0}(0)+D_{11}^m F_{11}^{\prime\pm1}(0)+G_{22}^m F_{22}^{\prime 0}(0)+D_{22}^m F_{22}^{\prime\pm1}(0)+E_{22}^m F_{22}^{\prime\pm2}(0)+D_{12}^m F_{12}^{\prime 1}(0)]. \tag{27}$$

The right-hand side of Eq. (26) is equal to that of Eq. (27) identically in regard to $a_{L_1L_2}^{(2n)}$, $a_{L_1L_2}^{\prime(2n)}$ and θ. From these conditions we obtain the following relations between sums. For simplicity we write $g_{11}G_{11}$ etc. for $\sum_m g_{11}^m G_{11}^m$ etc.

$$g_{11}G_{11}=(1/2)(d_{11}D_{11}-d_{11}G_{11}),\quad g_{11}D_{11}=d_{11}G_{11},$$
$$g_{22}G_{11}=(1/6)(5d_{22}G_{11}-d_{22}D),\quad g_{22}D_{11}=(1/3)(2d_{22}D_{11}-d_{22}G_{11}),$$
$$e_{22}G_{11}=d_{22}D_{11}-d_{22}G_{11},\quad e_{22}D_{11}=2d_{22}G_{11},$$
$$g_{11}G_{22}=(1/6)(5g_{11}D_{22}-d_{11}D_{22}),\quad g_{11}E_{22}=d_{11}D_{22}-g_{11}D_{22},$$
$$d_{11}G_{22}=(1/3)(2d_{11}D_{22}-g_{11}D_{22}),\quad d_{11}E_{22}=2g_{11}D_{22},$$
$$g_{22}G_{22}=(1/4)(2d_{22}D_{22}-d_{22}E_{22}),\quad g_{22}D_{22}=d_{22}G_{22},$$
$$g_{22}E_{22}=e_{22}G_{22}=(1/4)(-2d_{22}G_{22}+3d_{22}E_{22}),$$
$$e_{22}D_{22}=d_{22}E_{22},\quad e_{22}E_{22}=(1/4)(6d_{22}G_{22}+4d_{22}D_{22}-3d_{22}E_{22}),$$
$$g_{11}D_{12}=-d_{11}D_{12},$$
$$d_{12}G_{11}=-d_{12}D_{11},$$
$$g_{22}D_{12}=d_{22}D_{12}=-(1/2)e_{22}D_{12},$$
$$d_{12}G_{22}=d_{12}D_{22}=-(1/2)d_{12}E_{22}. \tag{28}$$

Inserting Eqs. (19), (20), (21) and (28) into Eq. (26), we obtain the following comparatively simple form of the angular correlation function,

$$\mathcal{W}(\theta)=[(3/2)a_{11}^{(0)}a_{11}^{\prime(0)}\{d_{11}G_{11}+d_{11}D_{11}\}+(5/2)a_{22}^{(0)}a_{11}^{\prime(0)}\{d_{22}G_{11}+d_{22}D_{11}\}$$
$$+(5/2)a_{11}^{(0)}a_{22}^{\prime(0)}\{g_{11}D_{22}+d_{11}D_{22}\}+(5/2)a_{22}^{(0)}a_{22}^{\prime(1)}\{d_{22}G_{22}+d_{22}D_{22}+d_{22}E_{22}\}]$$

$$+[3a_{11}^{(2)}a_{11}'^{(2)}\{-2d_{11}G_{11}+d_{11}D_{11}\}+7a_{22}^{(2)}a_{11}'^{(2)}\{2d_{22}G_{11}-d_{22}D_{11}\}$$
$$+7a_{11}^{(2)}a_{22}'^{(2)}\{2g_{11}D_{22}-d_{11}D_{22}\}+7a_{22}^{(2)}a_{22}'^{(2)}\{2d_{22}G_{22}+d_{22}D_{22}-2d_{22}E_{22}\}$$
$$+3a_{12}^{(2)}a_{11}'^{(2)}d_{12}D_{11}+3a_{11}^{(2)}a_{12}'^{(2)}d_{11}D_{12}+(7/2)a_{12}^{(2)}a_{22}'^{(2)}d_{12}E_{22}$$
$$+(7/2)a_{22}^{(2}a_{12}'^{(2)}e_{22}D_{12}+a_{12}^{(2)}a_{12}'^{(2)}d_{12}D_{12}]P_2(\cos\theta)$$
$$-[(35/4)a_{22}^{(4)}a_{22}'^{(4)}\{6d_{22}G_{22}-4d_{22}D_{22}+d_{22}E_{22}\}]P_4(\cos\theta). \qquad (29)$$

When the first transition involves $L=2$ and 3, and the second transition involves $L=1$ and 2, the relations between sums are besides Eq. (28)

$$g_{33}G_{11}=(1/10)(-f_{33}G_{11}+3f_{33}D_{11}),\quad g_{33}D_{11}=(1/5)(3f_{33}G_{11}+f_{33}D_{11}),$$
$$d_{33}G_{11}=(1/15)(-f_{33}G_{11}+8f_{33}D_{11}),\quad d_{33}D_{11}=(1/15)(16f_{33}G_{11}+7f_{33}D_{11}),$$
$$e_{33}G_{11}=(1/3)(f_{33}G_{11}+f_{33}D_{11}),\quad e_{33}D_{11}=(2/3)(f_{33}G_{11}+f_{33}D_{11}),$$
$$g_{33}G_{22}=(1/10)(5f_{33}G_{22}-3f_{33}D_{22}+3f_{33}E_{22}),$$
$$g_{33}D_{22}=(1/5)(-3f_{33}G_{22}+3f_{33}D_{22}+f_{33}E_{22}),$$
$$g_{33}E_{22}=(1/5)(3f_{33}G_{22}+f_{33}D_{22}),\quad d_{33}D_{22}=(1/5)(f_{33}G_{22}+2f_{33}E_{22}),$$
$$d_{33}D_{22}=(1/15)(7f_{33}D_{22}+8f_{33}E_{22}),$$
$$d_{33}E_{22}=(1/15)(12f_{33}G_{22}+8f_{33}D_{22}+f_{33}E_{22}),$$
$$e_{33}G_{22}=-f_{33}G_{22}+f_{33}D_{22},$$
$$e_{33}D_{22}=(1/3)(6f_{33}G_{22}-2f_{33}D_{22}+2f_{33}E_{22}),$$
$$e_{33}E_{22}=(1/3)(2f_{33}D_{22}+f_{33}E_{22}),$$
$$g_{33}D_{12}=-(2/5)f_{33}D_{12},\quad d_{33}D_{12}=-(3/5)f_{33}D_{12},\quad e_{33}D_{12}=0,$$
$$d_{23}G_{11}=-d_{23}D_{11}=-(2/\sqrt{10})e_{23}D_{11},\quad e_{23}G_{11}=-e_{23}D_{11},$$
$$d_{23}G_{22}=2d_{23}E_{22}-(5/\sqrt{10})e_{23}E_{22},\quad e_{23}G_{22}=(1/2)(-\sqrt{10}d_{23}E_{22}+e_{23}E_{22}),$$
$$d_{23}D_{22}=-3d_{23}E_{22}+(5/\sqrt{10})e_{23}E_{22},\quad e_{23}D_{22}=(1/2)(\sqrt{10}d_{23}E_{22}-3e_{23}E_{22}),$$
$$d_{23}D_{12}=(2/\sqrt{10})e_{23}D_{12}. \qquad (30)$$

The angular correlation function $\mathcal{W}(\theta)$ is

$$\mathcal{W}(\theta)=[(5/2)a_{22}^{(0)}a_{11}'^{(0)}\{d_{22}G_{11}+d_{22}D_{11}\}+(7/2)a_{33}^{(0}a_{11}'^{(0)}\{f_{33}G_{11}+f_{33}D_{11}\}$$
$$+(5/2)a_{22}^{(0)}a_{22}'^{(0)}\{d_{22}G_{22}+d_{22}D_{22}+d_{22}E_{22}\}$$
$$+(7/2)a_{33}^{(0)}a_{22}'^{(0)}\{f_{33}G_{22}+f_{33}D_{22}+f_{33}E_{22}\}]$$
$$+[7a_{22}^{(2)}a_{11}'^{(2)}\{2d_{22}G_{11}-d_{22}D_{11}\}-(42/5)a_{33}^{(2)}a_{11}'^{(2)}\{2f_{33}G_{11}-f_{33}D_{11}\}$$
$$+7a_{22}^{(2)}a_{22}'^{(2)}\{2d_{22}G_{22}+d_{22}D_{22}-2d_{22}E_{22}\}$$
$$-(42/5)a_{33}^{(2)}a_{22}'^{(2)}\{2f_{33}G_{22}+f_{33}D_{22}-2f_{33}E_{22}\}$$

$$+(7/2)a_{22}^{(2)}a_{12}'^{(2)}e_{22}D_{12}+(42/5)a_{33}^{(2)}a_{12}'^{(2)}f_{33}D_{12}+21a_{23}^{(2)}a_{11}'^{(2)}e_{23}D_{11}$$
$$+(7/2)a_{23}^{(2)}a_{22}'^{(2)}\{\sqrt{10}d_{23}E_{22}+5e_{23}E_{22}\}+7a_{23}^{(2)}a_{12}'^{(2)}e_{23}D_{12}]P_2(\cos\theta)$$
$$+[-(35/4)a_{22}^{(4)}a_{22}'^{(4)}\{6d_{22}G_{22}-4d_{22}D_{22}+d_{22}E_{22}\}$$
$$+(77/3)a_{33}^{(4)}a_{22}'^{(4)}\{6f_{33}G_{22}-4f_{33}D_{22}+f_{33}E_{22}\}$$
$$-35a_{23}^{(4)}a_{22}'^{(4)}\{\sqrt{10}d_{23}E_{22}-2e_{23}E_{22}\}]P_4(\cos\theta). \qquad (31)$$

The independent sums that appear in Eqs. (29) and (31) can be calculated with the table of Condon and Shortley[14] and the Appendix.

§ 3. Angular distribution functions of β-ray

In this section we calculate the explicit forms of the angular distribution functions defined by Eq. (11) for the β-rays up to the second forbidden. We treat each five interaction type of the Fermi theory separately and do not consider the case of mixed interaction types.

The angular distribution functions are obtained as follows. At first we calculate the matrix elements of the interaction Hamiltonian corresponding to the definite change of the magnetic quantum number of the nucleus. We denote them with $H_{\varkappa m}$, where $\varkappa$ and m are the quantum numbers of the emitted electron. Neglecting the common factor, the asymptotic wave function of the emitted electron is[15]

$$\psi=\sum_{\varkappa,m}H_{\varkappa m}\psi_{\varkappa m}. \qquad (32)$$

$\psi_{\varkappa m}$ are obtained by extracting the out-going waves, the parts containing $\exp(ikr)$, from the asymptotic forms of the eigenfunctions (standing waves) that contain the trigonometrical functions. We construct $\psi^*\psi$ from Eq. (32), sum over all the neutrino states and compare with Eq. (12), then the angular distribution functions are obtained.

We assume that the neutrino mass is zero. Then the Hamiltonian of a free neutrino commutes with γ_5. (We take $\gamma_5=-i\alpha_x\alpha_y\alpha_z$ as Konopinski and Uhlenbeck.[16] From this fact the angular distribution for any nuclear matrix element is the same as that for the nuclear matrix element which is obtained from the former by exchanging 1 for γ_5 and α for σ simultaneously. For example the angular distributions for $|\mathfrak{M}(A_{ij}^{\beta})|^2$ and $|\mathfrak{M}(B_{ij}^{\beta})|^2$ are the same. The angular distribution function for any nuclear matrix element containing β (Dirac matrix) is obtained from the angular distribution function for that without β by replacing K (neutrino energy) by $-K$.

We use the following properties of the phases of the nuclear matrix elements. The reduced nuclear matrix elements for the β-decay defined by Eq. (7) are divided into two classes; the nuclear matrix elements belonging to the same class have the same phase (or phase difference π), and the phase differences between those belonging to the different classes are $\pi/2$ (or $3\pi/2$). Up to the second forbidden the two classes are as follows: the one consists of $\mathfrak{M}(1)$, $\mathfrak{M}(\beta)$, $\mathfrak{M}(\gamma_5)$, $\mathfrak{M}(\beta\gamma_5)$, $\mathfrak{M}(\sigma)$, $\mathfrak{M}(\beta\sigma)$, $\mathfrak{M}(\alpha)$, $\mathfrak{M}(\beta\alpha)$, $\mathfrak{M}(\sigma\times r)$, $\mathfrak{M}(\beta\sigma\times r)$, $\mathfrak{M}(\alpha\times r)$, $\mathfrak{M}(R_{ij})$, $\mathfrak{M}(R_{ij}^{\beta})$, $\mathfrak{M}(S_{ijk})$, $\mathfrak{M}(S_{ijk}^{\beta})$ and the other

consists of $\mathfrak{M}(\boldsymbol{\sigma}\cdot\boldsymbol{r})$, $\mathfrak{M}(\beta\boldsymbol{\sigma}\cdot\boldsymbol{r})$, $\mathfrak{M}(\beta\boldsymbol{\alpha}\cdot\boldsymbol{r})$, $\mathfrak{M}(\boldsymbol{r})$, $\mathfrak{M}(\beta\boldsymbol{r})$, $\mathfrak{M}(B_{ij})$, $\mathfrak{M}(B_{ij}^{\beta})$, $\mathfrak{M}(A_{ij})$, $\mathfrak{M}(A_{ij}^{\beta})$, $\mathfrak{M}(T_{ij})$, $\mathfrak{M}(T_{ij}^{\beta})$. For the tensors of the same rank the proof has already been given by Longmire and Messiah.[17] For the tensors of the different ranks the proof is almost the same.

As an example, we consider A_{ij}^{β} and S_{ijk}^{β}. By the time reversal ($\mathfrak{K}$ is the time reversal operator), the wave functions Φ_J^M and $\Psi_{J'}^{M'}$, (J and J' are the total angular momenta, and M and M' are their z-components). and the operators* A_{ij}^{β} and S_{ijk}^{β} transform as follows:

$$\mathfrak{K}\Phi_J^M = e^{i\varphi}\Phi_J^{-M}, \qquad \mathfrak{K}\Psi_{J'}^{M'} = e^{i\psi}\Psi_{J'}^{-M'},$$

$$\mathfrak{K}A_{ij}^{\beta}\mathfrak{K}^{-1} = -A_{ij}^{\beta}, \quad \mathfrak{K}S_{ijk}^{\beta}\mathfrak{K}^{-1} = -S_{ijk}^{\beta}, \tag{33}$$

where φ and ψ are arbitrary phases. The operator $\mathfrak{K}$ can be represented as follows:

$$\mathfrak{K} = U\mathfrak{K}_0 \tag{34}$$

where $\mathfrak{K}_0$ transforms the wave function into its complex conjugate and U is a unitary operator. From Eqs. (33) and (34)

$$\begin{aligned} A_{ij}^{\beta MM'} &\equiv \langle \Psi_{J'}^{M'} | A_{ij}^{\beta} | \Phi_J^M \rangle = \langle \mathfrak{K}\Psi_{J'}^{M'}, \mathfrak{K}A_{ij}^{\beta}\mathfrak{K}^{-1}\mathfrak{K}\Phi_J^M \rangle^* \\ &= -e^{i(\psi-\varphi)}\langle \Psi_{J'}^{-M'} | A_{ij}^{\beta} | \Phi_J^{-M} \rangle^* \\ &\equiv -e^{i(\psi-\varphi)} A_{ij}^{\beta -M-M'*}. \end{aligned} \tag{35}$$

Similarly

$$S_{ijk}^{\beta MM'} = -e^{i(\psi-\varphi)} S_{ijk}^{\beta -M-M'*} \tag{36}$$

On the other hand the transformation coefficients have the following relations:

$$(JLmM|JLJ'm') = (-1)^{J'-J-L}(JL-m-M|JLJ'-m'). \tag{37}$$

Comparing Eqs. (7), (35), (36) and (37), we obtain

$$\frac{\mathfrak{M}(A_{ij}^{\beta})}{\mathfrak{M}(S_{ijk}^{\beta})} = -\frac{\mathfrak{M}^*(A_{ij}^{\beta})}{\mathfrak{M}^*(S_{ijk}^{\beta})}. \tag{38}$$

This indicates that the phases of $\mathfrak{M}(A_{ij}^{\beta})$ and $\mathfrak{M}(S_{ijk}^{\beta})$ are different by $\pi/2$ (or $3\pi/2$) from each other.

Using the above results we obtain the angular distribution functions:

1) Allowed

all isotropic.

2) 1st forbidden

a) scalar

$$\begin{aligned} F_{11}^{0}(\theta) = |\mathfrak{M}(\beta\boldsymbol{r})|^2 [&\{(1/3)K^2L_0 + (2/3)KN_0 + 2L_1 + M_0\} \\ &+ \{(4/3)KL_{12} + 2L_1 + 4N_{12}\} P_2(\cos\theta)]. \end{aligned} \tag{S1}$$

---

* Although Konopinski and Uhlenbeck[15] have used this notation for matrix elements, we use it here for operators.

b) vector

$$F_{11}^{0}(\theta)=|\mathfrak{M}(\boldsymbol{\alpha})|^2 L_0+|\mathfrak{M}(\boldsymbol{r})|^2[\{(1/3)K^2L_0-(2/3)KN_0+2L_1+M_0\}$$
$$+\{-(4/3)KL_{12}+2L_1+4N_{12}\}P_2(\cos\theta)]$$
$$-\{i\mathfrak{M}^*(\boldsymbol{\alpha})\mathfrak{M}(\boldsymbol{r})+\text{c.c.}\}[\{(1/3)KL_0-N_0\}-2L_{12}P_2(\cos\theta)]. \quad \text{(V1)}$$

c) tensor

$$F_{00}^{0}(\theta)=|\mathfrak{M}(\beta\boldsymbol{\sigma}\cdot\boldsymbol{r})|^2[(1/9)K^2L_0+(2/3)KN_0+M_0],$$
$$F_{11}^{0}(\theta)=|\mathfrak{M}(\beta\boldsymbol{\alpha})|^2 L_0+|\mathfrak{M}(\beta\boldsymbol{\sigma}\times\boldsymbol{r})|^2[\{(1/6)K^2L_0-(2/3)KN_0+(1/2)L_1+M_0\}$$
$$+\{(2/3)KL_{12}+(1/2)L_1-2N_{12}\}P_2(\cos\theta)]$$
$$-\{\mathfrak{M}^*(\beta\boldsymbol{\alpha})\mathfrak{M}(\beta\boldsymbol{\sigma}\times\boldsymbol{r})+\text{c.c.}\}[\{(1/3)KL_0-N_0\}+L_{12}P_2(\cos\theta)],$$
$$F_{22}^{0}(\theta)=|\mathfrak{M}(B_{ij}^{3})|^2[\{(1/12)K^2L_0+(3/4)L_1\}+(3/4)L_1P_2(\cos\theta)],$$
$$F_{02}^{0}(\theta)=\{\mathfrak{M}^*(\beta\boldsymbol{\sigma}\cdot\boldsymbol{r})\mathfrak{M}(B_{ij}^{3})+\text{c.c.}\}(1/\sqrt{6})\{KL_{12}+3N_{12}\}P_2(\cos\theta),$$
$$F_{12}^{1}(\theta)=-\{i\mathfrak{M}^*(\beta\boldsymbol{\alpha})\mathfrak{M}(B_{ij}^{3})+\text{c.c.}\}\{3/(2\sqrt{2})\}L_{12}P_2(\cos\theta)$$
$$-\{i\mathfrak{M}^*(\beta\boldsymbol{\sigma}\times\boldsymbol{r})\mathfrak{M}(B_{ij}^{3})+\text{c.c.}\}$$
$$\cdot(1/\sqrt{2})\{-(1/2)KL_{12}+(3/4)L_1+(3/2)N_{12}\}P_2(\cos\theta). \quad \text{(T1)}$$

d) pseudovector

$$F_{00}^{0}(\theta)=|\mathfrak{M}(\gamma_5)|^2 L_0+|\mathfrak{M}(\boldsymbol{\sigma}\cdot\boldsymbol{r})|^2[(1/9)K^2L_0-(2/3)KN_0+M_0]$$
$$-\{i\mathfrak{M}^*(\gamma_5)\mathfrak{M}(\boldsymbol{\sigma}\cdot\boldsymbol{r})+\text{c.c.}\}[(1/3)KL_0-N_0],$$
$$F_{11}^{0}(\theta)=|\mathfrak{M}(\boldsymbol{\sigma}\times\boldsymbol{r})|^2[\{(1/6)K^2L_0+(2/3)KN_0+(1/2)L_1+M_0\}$$
$$+\{-(2/3)KL_{12}+(1/2)L_1-2N_{12}\}]P_2(\cos\theta),$$
$$F_{22}^{0}(\theta)=|\mathfrak{M}(B_{ij})|^2[\{1/12\}K^2L_0+(3/4)L_1\}+(3/4)L_1P_2(\cos\theta)],$$
$$F_{02}^{0}(\theta)=\{i\mathfrak{M}^*(\gamma_5)\mathfrak{M}(B_{ij})+\text{c.c.}\}(\sqrt{3}/\sqrt{2})L_{12}P_2(\cos\theta)$$
$$+\{\mathfrak{M}^*(\boldsymbol{\sigma}\cdot\boldsymbol{r})\mathfrak{M}(B_{ij})+\text{c.c.}\}(1/\sqrt{6})\{-KL_{12}+3N_{12}\}P_2(\cos\theta),$$
$$F_{12}^{1}(\theta)=-\{i\mathfrak{M}^*(\boldsymbol{\sigma}\times\boldsymbol{r})\mathfrak{M}(B_{ij})+\text{c.c.}\}$$
$$\cdot(1/\sqrt{2})\{(1/2)KL_{12}+(3/4)L_1+(3/2)N_{12}\}P_2(\cos\theta). \quad \text{(A1)}$$

e) pseudoscalar (We define $\mathfrak{M}(\beta\gamma_5)$ as the 1st forbidden).

$$F_{00}^{0}(\theta)=|\mathfrak{M}(\beta\gamma_5)|^2 L_0. \quad \text{(P1)}$$

3) 2nd forbidden

a) scalar

$$F_{22}^{0}(\theta)=|\mathfrak{M}(R_{ij}^{3})|^2[\{(1/30)K^4L_0+(2/15)K^3N_0+(2/3)K^2L_1+(1/3)K^2M_0$$
$$+2KN_1+(9/2)L_2+3M_1\}+\{(2/15)K^3L_{12}+(1/3)K^2L_1+(2/3)K^2N_{12}$$

$$+(6/7)KL_{23}+2KN_1+(36/7)L_2+3M_1+(18/7)N_{23}\}\ P_2(\cos\theta)$$
$$+\{(36/7)KL_{23}+(27/7)L_2+(108/7)N_{23}\}\ P_4(\cos\theta)]\,. \qquad \text{(S2)}$$

b) vector

$$F_{11}^0(\theta)=|\mathfrak{M}(\boldsymbol{\alpha}\times\boldsymbol{r})|^2[\{(1/6)K^2L_0+(2/3)KN_0+(1/2)L_1+M_0\}$$
$$+\{-(2/3)KL_{12}+(1/2)L_1-2N_{12}\}\ P_2(\cos\theta)],$$
$$F_{22}^0(\theta)=|\mathfrak{M}(A_{ij})|^2[\{(1/12)K^2L_0+(3/4)L_1\}+(3/4)L_1P_2(\cos\theta)]$$
$$+|\mathfrak{M}(R_{ij})|^2[\{(1/30)K^4L_0-(2/15)K^3N_0+(2/3)K^2L_1+(1/3)K^2M_0$$
$$-2KN_1+(9/2)L_2+3M_1\}+\{-(2/15)K^3L_{12}+(1/3)K^2L_1+(2/3)K^2N_{12}$$
$$-(6/7)KL_{23}-2KN_1+(36/7)L_2+3M_1+(18/7)N_{23}\}\ P_2(\cos\theta)$$
$$+\{-(36/7)KL_{23}+(27/7)L_2+(108/7)N_{23}\}\ P_4(\cos\theta)]$$
$$-\{i\mathfrak{M}^*(A_{ij})\mathfrak{M}(R_{ij})+\text{c.c.}\}[\{(1/30)K^3L_0$$
$$-(1/6)K^2N_0+(1/2)KL_1-(3/2)N_1\}$$
$$+\{-(1/6)K^2L_{12}+(1/2)KL_1-(9/14)L_{23}-(3/2)N_1\}\ P_2(\cos\theta)$$
$$-(27/7)L_{23}P_4(\cos\theta)],$$
$$F_{12}^1(\theta)=-\{i\mathfrak{M}^*(\boldsymbol{\alpha}\times\boldsymbol{r})\mathfrak{M}(A_{ij})+\text{c.c.}\}(1/\sqrt{2})\{(1/2)KL_{12}$$
$$+(3/4)L_1+(3/2)N_{12}\}\ P_2(\cos\theta)$$
$$-\{\mathfrak{M}^*(\boldsymbol{\alpha}\times\boldsymbol{r})\mathfrak{M}(R_{ij})+\text{c.c.}\}(1/\sqrt{2})\{(1/2)K^2L_{12}+(1/2)KL_1-KL_{13}$$
$$+KN_{12}+KN_{21}+(3/2)L_{23}+3M_{12}-(3/2)N_1-3N_{13}\}\ P_2(\cos\theta). \qquad \text{(V2)}$$

c) tensor

$$F_{00}^0(\theta)=|\mathfrak{M}(\beta\boldsymbol{\alpha}\cdot\boldsymbol{r})|^2\ \{(1/9)K^2L_0+(2/3)KN_0+M_0\},$$
$$F_{22}^0(\theta)=|\mathfrak{M}(A_{ij}^{\beta})|^2[\{(1/12)K^2L_0+(3/4)L_1\}+(3/4)L_1P_2(\cos\theta)]$$
$$+|\mathfrak{M}(T_{ij}^{\beta})|^2(1/12)[\{(1/15)K^4L_0-(2/5)K^3N_0+K^2L_1+K^2M_0$$
$$-6KN_1+6L_2+9M_1\}+\{K^2L_1+(12/7)KL_{23}-6KN_1+(48/7)L_2$$
$$+9M_1-(36/7)N_{23}\}\ P_2(\cos\theta)$$
$$+\{(72/7)KL_{23}+(36/7)L_2-(216/7)N_{23}\}\ P_4(\cos\theta)]$$
$$-\{\mathfrak{M}^*(A_{ij}^{\beta})\mathfrak{M}(T_{ij}^{\beta})+\text{c.c.}\}(1/4)[\{(1/15)K^3L_0$$
$$-(1/3)K^2N_0+KL_1-3N_1\}$$
$$+\{KL_1+(6/7)L_{23}-3N_1\}\ P_2(\cos\theta)+(36/7)L_{23}P_4(\cos\theta)],$$
$$F_{33}^0(\theta)=|\mathfrak{M}(S_{ijk}^{\beta})|^2(1/72)[\{(1/15)K^4L_0+2K^2L_1+15L_2\}$$
$$+\{(8/5)K^2L_1+(120/7)L_2\}\ P_2(\cos\theta)+(90/7)L_2P_4(\cos\theta)],$$

$$F_{23}^{1}(\theta)=-\{i\mathfrak{M}^{*}(A_{ij}^{\beta})\mathfrak{M}(S_{ijk}^{\beta})+\text{c.c.}\}\,(\sqrt{10}/\sqrt{3})[\{(1/60)K^{2}L_{12}$$
$$+(3/28)L_{23}\}\,P_{2}(\cos\theta)+(15/56)L_{23}P_{4}(\cos\theta)]$$
$$-\{i\mathfrak{M}^{*}(T_{ij}^{\beta})\mathfrak{M}(S_{ijk}^{\beta})+\text{c.c.}\}\,(\sqrt{10}/\sqrt{3})[\{(1/300)(-K^{3}L_{12}$$
$$+5K^{2}N_{12})+(1/28)(-KL_{23}+2L_{2}+3N_{23})\}\,P_{2}(\cos\theta)$$
$$+(5/56)\{-KL_{23}+2L_{2}+3N_{23}\}\,P_{4}(\cos\theta)]\,. \qquad \text{(T2)}$$

d) pseudovector

$$F_{22}^{0}(\theta)=|\mathfrak{M}(T_{ij})|^{2}(1/12)[\{(1/15)K^{4}L_{0}+(2/5)K^{3}N_{0}+K^{2}L_{1}+K^{2}M_{0}$$
$$+6KN_{1}+6L_{1}+9M_{1}\}+\{K^{2}L_{1}-(12/7)KL_{23}+6KN_{1}+(48/7)L_{2}$$
$$+9M_{1}-(36/7)N_{23}\}\,P_{2}(\cos\theta)$$
$$+\{-(72/7)KL_{23}+(36/7)L_{2}-(216/7)N_{23}\}\,P_{4}(\cos\theta)];$$
$$F_{33}^{0}(\theta)=|\mathfrak{M}(S_{ijk})|^{2}(1/72)[\{(1/15)K^{4}L_{0}+2K^{2}L_{1}+15L_{2}\}$$
$$+\{(8/5)K^{2}L_{1}+(120/7)L_{2}\}\,P_{2}(\cos\theta)+(90/7)L_{2}P_{4}(\cos\theta)],$$
$$F_{23}^{1}(\theta)=-\{i\mathfrak{M}^{*}(T_{ij})\mathfrak{M}(S_{ijk})+\text{c.c.}\}\,(\sqrt{10}/\sqrt{3})[\{(1/300)(K^{3}L_{12}+5K^{2}N_{12})$$
$$+(1/28)(KL_{23}+2L_{2}+3N_{23})\}\,P_{2}(\cos\theta)$$
$$+(5/56)\{KL_{23}+2L_{2}+3N_{23}\}\,P_{4}(\cos\theta)]. \qquad \text{(A2)}$$

e) pseudoscalar

$$F_{11}^{0}(\theta)=|\mathfrak{M}(\beta\gamma_{5}\boldsymbol{p}^{\nu})|^{2}[\{(1/3)K^{2}L_{0}+(2/3)KN_{0}+2L_{1}+M_{0}\}$$
$$+\{(4/3)KL_{12}+2L_{1}+4N_{12}\}\,P_{2}(\cos\theta)]\,. \qquad \text{(P2)}$$

The notation is almost the same as that of Konopinski and Uhlenbeck,[16] but we write β explicitly for the nuclear matrix elements including it. Moreover, we use the following new notation, which is necessary to describe the interference terms between different $\psi_{\varkappa m}$'s.

$$L_{12}=\left(\frac{p^{2}}{2\pi}F\right)^{-1}\frac{g_{-1}f_{2}\cos(\delta_{-1}-\delta_{2})-f_{1}g_{-2}\cos(\delta_{1}-\delta_{-2})}{4\pi\rho}$$
$$\to-\frac{p^{2}}{3W},$$
$$L_{13}=\left(\frac{p^{2}}{2\pi}F\right)^{-1}\frac{g_{-1}g_{-3}\cos(\delta_{-1}-\delta_{-3})+f_{1}f_{3}\cos(\delta_{1}-\delta_{3})}{4\pi\rho^{2}}$$
$$\to-\frac{p^{2}}{15},$$
$$L_{23}=\left(\frac{p^{2}}{2\pi}F\right)^{-1}\frac{g_{-2}f_{3}\cos(\delta_{-2}-\delta_{3})-f_{2}g_{-3}\cos(\delta_{2}-\delta_{-3})}{4\pi\rho^{3}}$$
$$\to-\frac{p^{4}}{45W},$$

$$M_{12}=\left(\frac{p^2}{2\pi}F\right)^{-1}\frac{f_{-1}g_2\cos(\delta_{-1}-\delta_2)-g_1f_{-2}\cos(\delta_1-\delta_{-2})}{4\pi\rho^3}$$

$$\rightarrow\frac{p^4}{45W}+\frac{p^2}{6W}\frac{\alpha^2Z^2}{4\rho^2}+\frac{11}{90}\frac{p^2}{2}\frac{\alpha Z}{\rho},$$

$$N_{12}=\left(\frac{p^2}{2\pi}F\right)^{-1}\frac{f_{-1}f_2\cos(\delta_{-1}-\delta_2)+g_1g_{-2}\cos(\delta_1-\delta_{-2})}{4\pi\rho^2}$$

$$\rightarrow\frac{p^2}{9}+\frac{p^2}{3W}\frac{\alpha Z}{2\rho},$$

$$N_{21}=\left(\frac{p^2}{2\pi}F\right)^{-1}\frac{g_{-1}g_2\cos(\delta_{-1}-\delta_2)+f_1f_{-2}\cos(\delta_1-\delta_{-2})}{4\pi\rho^2}$$

$$\rightarrow-\frac{p^2}{15}-\frac{p^2}{6W}\frac{\alpha Z}{2\rho},$$

$$N_{13}=\left(\frac{p^2}{2\pi}F\right)^{-1}\frac{f_{-1}g_{-3}\cos(\delta_{-1}-\delta_{-3})-g_1f_3\cos(\delta_1-\delta_3)}{4\pi\rho^3}$$

$$\rightarrow\frac{p^4}{45W}+\frac{p^2}{15}\frac{\alpha Z}{2\rho};$$

$$N_{23}=\left(\frac{p^2}{2\pi}F\right)^{-1}\frac{f_{-2}f_3\cos(\delta_{-2}-\delta_3)+g_2g_{-3}\cos(\delta_2-\delta_{-3})}{4\pi\rho^4}$$

$$\rightarrow\frac{p^4}{225}+\frac{p^4}{90W}\frac{\alpha Z}{2\rho}. \qquad (39)$$

In the above definition we mainly follow the notation of Konopinski and Uhlenbeck[16] and Rose,[18] but it should be noted that the suffixes of f and g are not those of Rose[18] but quantum numbers $\varkappa$. It is more natural and convenient to use the suffixes $\varkappa$. The relation between the two suffixes is shown in Table I. $\delta_\varkappa$ are the phases of the asymptotic wave functions. $\rightarrow$denotes the approximation which is valid for $\alpha ZW/p\ll 1$. When this approximation can not be used, the calculation of Eq. (39) is considerably complicated, and moreover, for the heavy nuclei it is necessary to change $f_\varkappa$ and $g_\varkappa$ from the Coulomb wave functions and to take into account the effect of the finite nuclear size.[15] As usual the values of $f_\varkappa$ and $g_\varkappa$ are to be taken at $r=\rho$. (ρ is the nuclear radius.) From Eq. (39) it can be understood that M_{ij} and N_{ij} are strongly affected by the Coulomb field.

Suffixes of Rose[18]	2	1	0	−2	−3	−4
$\varkappa$	−3	−2	−1	1	2	3

Table I

Finally we mention about the relation between the reduced nuclear matrix elements used here and the nuclear matrix elements used commonly in the theory of β-spectra. The latter ones have the forms of

$$\sum_{i_1,\cdots i_L}\sum_{m'}(J'm'|T_{i_1,\cdots i_L}|Jm)^*(J'm'|T'_{i_1,\cdots i_L}|Jm).$$

By Eq. (6) this equals to

$$\sum_{M}\sum_{m'}(J'm'|\mathcal{H}_{LM}|Jm)^*(J'm'|\mathcal{H}'_{LM}|Jm).$$

By Eq. (7) this equals to

$$\mathfrak{M}^*(T_{i_1\cdots i_L})\mathfrak{M}(T'_{i_1\cdots i_L})\sum_{m'}(JLmM|JLJ'm')^2$$
$$=(2J'+1)/(2J+1)\cdot\mathfrak{M}^*(T_{i_1\cdots i_L})\mathfrak{M}(T'_{i_1\cdots i_L}).$$

For example,

$$\sum A^{\beta*}_{ij}T^{\beta}_{ij}=(2J'+1)/(2J+1)\cdot\mathfrak{M}^*(A^{\beta}_{ij})\mathfrak{M}(T^{\beta}_{ij}).$$

$(2J'+1)/(2J+1)$ is common to all the terms, so that this factor need not be considered in the angular correlation. Therefore, when we study the β-spectra the factors such as $\sum A^{\beta*}_{ij}T^{\beta}_{ij}$ may be replaced by the factors such as $\mathfrak{M}^*(A^{\beta}_{ij})\mathfrak{M}(T^{\beta}_{ij})$.

Comparison with the experiments will be reported in the subsequent paper.

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Appendix

We calculate the transformation coefficients $(j_1 3 m_1 m_2|j_1 3 jm)$, using the formula in reference 14 p. 75 :

$$(j_1 j_2 m_1 m_2|j_1 j_2 jm)=\delta(m,m_1+m_2)$$
$$\cdot\sqrt{\frac{(j+j_1-j_2)!\,(j-j_1+j_2)!\,(j_1+j_2-j)!\,(j+m)!\,(j-m)!\,(2j+1)}{(j+j_1+j_2+1)!\,(j_1-m_1)!\,(j_1+m_1)!\,(j_2-m_2)!\,(j_2+m_2)!}}$$
$$\cdot\sum_{x}\frac{(-1)^{x+j_2+m_2}(j+j_2+m_1-x)!\,(j_1-m_1+x)!}{(j-j_1+j_2-x)!\,(j+m-x)!\,x!\,(x+j_1-j_2-m)!}.$$

The results are shown in the following table.

$$(j_1 3 m_1 m_2|j_1 3 jm)$$

$j=j_1+3$,

$$m_2=3,\ \sqrt{\frac{(j_1+m-2)(j_1+m-1)(j_1+m)(j_1+m+1)(j_1+m+2)(j_1+m+3)}{(2j_1+1)(2j_1+2)(2j_1+3)(2j_1+4)(2j_1+5)(2j_1+6)}}$$

$$m_2=2,\ \sqrt{6}\sqrt{\frac{(j_1-m+3)(j_1+m-1)(j_1+m)(j_1+m+1)(j_1+m+2)(j_1+m+3)}{(2j_1+1)(2j_1+2)(2j_1+3)(2j_1+4)(2j_1+5)(2j_1+6)}}$$

$$m_2=1,\ \sqrt{15}\sqrt{\frac{(j_1-m+3)(j_1-m+2)(j_1+m)(j_1+m+1)(j_1+m+2)(j_1+m+3)}{(2j_1+1)(2j_1+2)(2j_1+3)(2j+4)(2j_1+5)(2j_1+6)}}$$

$$m_2=0,\ \sqrt{20}\sqrt{\frac{(j_1-m+3)(j_1-m+2)(j_1-m+1)(j_1+m+1)(j_1+m+2)(j_1+m+3)}{(2j_1+1)(2j_1+2)(2j_1+3)(2j+4)(2j+5)(2j+6)}}$$

$$m_2=-1,\ \sqrt{15}\sqrt{\frac{(j_1-m+3)(j_1-m+2)(j_1-m+1)(j_1-m)(j_1+m+2)(j_1+m+3)}{(2j_1+1)(2j_1+2)(2j_1+3)(2j_1+4)(2j_1+5)(2j_1+6)}}$$

$$m_2=-2,\ \sqrt{6}\sqrt{\frac{(j_1-m+3)(j_1-m+2)(j_1-m+1)(j_1-m)(j_1-m-1)(j_1+m+3)}{(2j_1+1)(2j_1+2)(2j_1+3)(2j_1+4)(2j_1+5)(2j_1+6)}}$$

$$m_2=-3,\ \sqrt{\frac{(j_1-m+3)(j_1-m+2)(j_1-m+1)(j_1-m)(j_1-m-1)(j_1-m-2)}{(2j_1+1)(2j_1+2)(2j_1+3)(2j_1+4)(2j_1+5)(2j_1+6)}}$$

$j=j_1+2$

$$m_2=3,\ -\sqrt{6}\sqrt{\frac{(j_1-m+3)(j_1+m-2)(j_1+m-1)(j_1+m)(j_1+m+1)(j_1+m+2)}{2j_1(2j_1+1)(2j_1+2)(2j_1+3)(2j_1+4)(2j_1+6)}}$$

$$m_2=2,\ -2(2j_1-3m+6)\sqrt{\frac{(j_1+m-1)(j_1+m)(j_1+m+1)(j_1+m+2)}{2j_1(2j_1+1)(2j_1+2)(2j_1+3)(2j_1+4)(2j_1+6)}}$$

$$m_2=1,\ -\sqrt{10}(j_1-3m+3)\sqrt{\frac{(j_1-m+2)(j_1+m)(j_1+m+1)(j_1+m+2)}{2j_1(2j_1+1)(2j_1+2)(2j_1+3)(2j_1+4)(2j_1+6)}}$$

$$m_2=0,\ 2\sqrt{30}m\sqrt{\frac{(j_1-m+2)(j_1-m+1)(j_1+m+1)(j_1+m+2)}{2j_1(2j+1)(2j_1+2)(2j_1+3)(2j_1+4)(2j_1+6)}}$$

$$m_2=-1,\ \sqrt{10}(j_1+3m+3)\sqrt{\frac{(j_1-m+2)(j_1-m+1)(j_1-m)(j_1+m+2)}{2j_1(2j_1+1)(2j_1+2)(2j_1+3)(2j_1+4)(2j_1+6)}}$$

$$m_2=-2,\ 2(2j_1+3m+6)\sqrt{\frac{(j_1-m+2)(j_1-m+1)(j_1-m)(j_1-m-1)}{2j_1(2j_1+1)(2j_1+2)(2j_1+3)(2j_1+4)(2j_1+6)}}$$

$$m_2=-3,\ \sqrt{6}\sqrt{\frac{(j_1-m+2)(j_1-m+1)(j_1-m)(j_1-m-1)(j_1-m-2)(j_1+m+3)}{2j_1(2j_1+1)(2j_1+2)(2j_1+3)(2j_1+4)(2j_1+6)}}$$

$j=j_1+1$

$$m_2=3,\ \sqrt{15}\sqrt{\frac{(j_1-m+3)(j_1-m+2)(j_1+m-2)(j_1+m-1)(j_1+m)(j_1+m+1)}{(2j_1-1)2j_1(2j_1+1)(2j_1+2)(2j_1+4)(2j_1+5)}}$$

$$m_2=2,\ \sqrt{10}(j_1-3m+4)\sqrt{\frac{(j_1-m+2)(j_1+m-1)(j_1+m)(j_1+m+1)}{(2j_1-1)2j_1(2j_1+1)(2j_1+2)(2j_1+4)(2j_1+5)}}$$

$$m_2=1,$$
$$-(j_1^2+10j_1m-15m^2-3j_1+25m-10)\sqrt{\frac{(j_1+m)(j_1+m+1)}{(2j_1-1)2j_1(2j_1+1)(2j_1+2)(2j_1+4)(2j_1+5)}}$$

$$m_2=0,\ -2\sqrt{3}(j_1^2-5m^2+2j_1)\sqrt{\frac{(j_1-m+1)(j_1+m+1)}{(2j_1-1)2j_1(2j_1+1)(2j_1+2)(2j_1+4)(2j_1+5)}}$$

$$m_2=-1,\ -(j_1^2-10j_1m-15m^2-3j_1-25m-10)\cdot\sqrt{\frac{(j_1-m+1)(j_1-m)}{(2j_1-1)2j_1(2j_1+1)(2j_1+2)(2j_1+4)(2j_1+5)}}$$

$$m_2=-2,\ \sqrt{10}(j_1+3m+4)\sqrt{\frac{(j_1-m+1)(j_1-m)(j_1-m-1)(j_1+m+2)}{(2j_1-1)2j_1(2j_1+1)(2j_1+2)(2j_1+4)(2j_1+5)}}$$

$$m_2=-3,\ \sqrt{15}\sqrt{\frac{(j_1+m+3)(j_1+m+2)(j_1-m-2)(j_1-m-1)(j_1-m)(j_1-m+1)}{(2j_1-1)2j_1(2j_1+1)(2j_1+2)(2j_1+4)(2j_1+5)}}$$

$j=j_1$

$$m_2=3,\ -2\sqrt{5}\sqrt{\frac{(j_1-m+3)(j_1-m+2)(j_1-m+1)(j_1+m)(j_1+m-1)(j_1+m-2)}{(2j_1-2)(2j_1-1)2j_1(2j_1+2)(2j_1+3)(2j_1+4)}}$$

$$m_2=2,\ 2(m-1)\sqrt{30}\sqrt{\frac{(j_1-m+2)(j_1-m+1)(j_1+m)(j_1+m-1)}{(2j_1-2)(2j_1-1)2j_1(2j_1+2)(2j_1+3)(2j_1+4)}}$$

$$m_2=1,\ 2\sqrt{2}[j_1(j_1+1)-5m(m-1)-2]\cdot\sqrt{\frac{(j_1-m+1)(j_1+m)}{(2j_1-2)(2j_1-1)2j_1(2j_1+2)(2j_1+3)(2j_1+4)}}$$

$$m_2=0,\ -4m(3j_1^2-5m^2+3j_1-1)\frac{1}{\sqrt{(2j_1-2)(2j_1-1)2j(2j_1+2)(2j_1+3)(2j_1+4)}}$$

$$m_2=-1,\ -2\sqrt{2}[j_1(j_1+1)-5m(m+1)-2]\cdot\sqrt{\frac{(j_1-m)(j_1+m+1)}{(2j_1-2)(2j_1-1)2j_1(2j_1+2)(2j_1+3)(2j_1+4)}}$$

$$m_2=-2,\ 2(m+1)\sqrt{30}\sqrt{\frac{(j_1-m)(j_1-m-1)(j_1+m+2)(j_1+m+1)}{(2j_1-2)(2j_1-1)2j_1(2j_1+2)(2j_1+3)(2j_1+4)}}$$

$$m_2=-3,\ 2\sqrt{5}\sqrt{\frac{(j_1-m)(j_1-m-1)(j_1-m-2)(j_1+m+3)(j_1+m+2)(j_1+m+1)}{(2j_1-2)(2j_1-1)2j_1(2j_1+2)(2j_1+3)(2j_1+4)}}$$

$j=j_1-1$

$$m_2=3,\ \sqrt{15}\sqrt{\frac{(j_1-m+3)(j_1-m+2)(j_1-m+1)(j_1-m)(j_1+m-1)(j_1+m-2)}{(2j_1-3)(2j_1-2)2j_1(2j_1+1)(2j_1+2)(2j_1+3)}}$$

$$m_2=2,\ -(j_1+3m-3)\sqrt{10}\sqrt{\frac{(j_1-m+2)(j_1-m+1)(j_1-m)(j_1+m-1)}{(2j_1-3)(2j_1-2)2j_1(2j_1+1)(2j_1+2)(2j_1+3)}}$$

$$m_2=1,\ (-j_1^2+10j_1m+15m^2-5j_1-15m+6)\cdot\sqrt{\frac{(j_1-m+1)(j_1-m)}{(2j_1-3)(2j_1-2)2j_1(2j_1+1)(2j_1+2)(2j_1+3)}}$$

$$m_2=0,\ (j_1^2-5m^2-1)\,2\sqrt{3}\sqrt{\frac{(j_1-m)(j_1+m)}{(2j_1-3)(2j_1-2)2j_1(2j_1+1)(2j_1+2)(2j_1+3)}}$$

$$m_2=-1,\ (-j_1^2-10j_1m+15m^2-5j_1+15m+6)$$
$$\cdot\sqrt{\frac{(j_1+m+1)(j_1+m)}{(2j_1-3)(2j_1-2)2j_1(2j_1+1)(2j_1+2)(2j_1+3)}}$$

$$m_2=-2,\ (-j_1+3m+3)\sqrt{10}\sqrt{\frac{(j_1-m-1)(j_1+m+2)(j_1+m+1)(j_1+m)}{(2j_1-3)(2j_1-2)2j_1(2j_1+1)(2j_1+2)(2j_1+3)}}$$

$$m_2=-3,\ \sqrt{15}\sqrt{\frac{(j_1-m-1)(j_1-m-2)(j_1+m+3)(j_1+m+2)(j_1+m+1)(j_1+m)}{(2j_1-3)(2j_1-2)2j_1(2j_1+1)(2j_1+2)(2j_1+3)}}$$

$j=j_1-2$

$$m_2=3,\ -\sqrt{6}\sqrt{\frac{(j_1-m+3)(j_1-m+2)(j_1-m+1)(j_1-m)(j_1-m-1)(j_1+m-2)}{(2j_1-4)(2j_1-2)(2j_1-1)2j_1(2j_1+1)(2j_1+2)}}$$

$$m_2=2,\ 2(2j_1+3m-4)\sqrt{\frac{(j_1-m+2)(j_1-m+1)(j-m)(j_1-m-1)}{(2j_1-4)(2j_1-2)(2j_1-1)\,2j_1(2j_1+1)(2j_1+2)}}$$

$$m_2=1,\ -(j_1+3m-2)\sqrt{10}\sqrt{\frac{(j_1-m+1)(j_1-m)(j_1-m-1)(j_1+m-1)}{(2j_1-4)(2j_1-2)(2j_1-1)\,2j_1(2j_1+1)(2j_1+2)}}$$

$$m_2=0,\ 2m\sqrt{30}\sqrt{\frac{(j_1-m)(j_1-m-1)(j_1+m)(j_1+m-1)}{(2j_1-4)(2j_1-2)(2j_1-1)2j_1(2j_1+1)(2j_1+2)}}$$

$$m_2=-1,\ (j_1-3m-2)\sqrt{10}\sqrt{\frac{(j_1-m-1)(j_1+m+1)(j_1+m)(j_1+m-1)}{(2j_1-4)(2j_1-2)(2j_1-1)2j_1(2j_1+1)(2j_1+2)}}$$

$$m_2=-2,\ -2(2j_1-3m-4)\sqrt{\frac{(j_1+m+2)(j_1+m+1)(j_1+m)(j_1+m-1)}{(2j_1-4)(2j_1-2)(2j_1-1)\,2j_1(2j_1+1)(2j_1+2)}}$$

$$m_2=-3,\ \sqrt{6}\sqrt{\frac{(j_1-m-2)(j_1+m+3)(j_1+m+2)(j_1+m+1)(j_1+m)(j_1+m-1)}{(2j_1-4)(2j_1-2)(2j_1-1)2j_1(2j_1+1)(2j_1+2)}}$$

$j=j_1-3$

$$m_2=3,\ \sqrt{\frac{(j_1-m+3)(j_1-m+2)(j_1-m+1)(j_1-m)(j_1-m-1)(j_1-m-2)}{(2j_1-4)(2j_1-3)(2j_1-2)(2j_1-1)2j_1(2j_1+1)}}$$

$$m_2=2,\ -\sqrt{6}\sqrt{\frac{(j_1-m+2)(j_1-m+1)(j_1-m)(j_1-m-1)(j_1-m-2)(j_1+m-2)}{(2j_1-4)(2j_1-3)(2j_1-2)(2j_1-1)2j_1(2j_1+1)}}$$

$$m_2=1,\ \sqrt{15}\sqrt{\frac{(j_1-m+1)(j_1-m)(j_1-m-1)(j_1-m-2)(j_1+m-1)(j_1+m-2)}{(2j_1-4)(2j_1-3)(2j_1-2)(2j_1-1)2j_1(2j_1+1)}}$$

$$m_2=0,\quad -\sqrt{20}\sqrt{\frac{(j_1-m)(j_1-m-1)(j_1-m-2)(j_1+m)(j_1+m-1)(j_1+m-2)}{(2j_1-4)(2j_1-3)(2j_1-2)(2j_1-1)2j_1(2j_1+1)}}$$

$$m_2=-1,\quad \sqrt{15}\sqrt{\frac{(j_1-m-1)(j_1-m-2)(j_1+m+1)(j_1+m)(j_1+m-1)(j_1+m-2)}{(2j_1-4)(2j_1-3)(2j_1-2)(2j_1-1)2j_1(2j_1+1)}}$$

$$m_2=-2,\quad -\sqrt{6}\sqrt{\frac{(j_1-m-2)(j_1+m+2)(j_1+m+1)(j_1+m)(j_1+m-1)(j_1+m-2)}{(2j_1-4)(2j_1-3)(2j_1-2)(2j_1-1)2j_1(2j_1+1)}}$$

$$m_2=-3,\quad \sqrt{\frac{(j_1+m+3)(j_1+m+2)(j_1+m+1)(j_1+m)(j_1+m-1)(j_1+m-2)}{(2j_1-4)(2j_1-3)(2j_1-2)(2j_1-1)2j_1(2j_1+1)}}.$$

References

1) D. R. Hamilton, Phys. Rev. **58** (1940), 122.
2) D. L. Falkoff and G. E. Uhlenbeck, Phys. Rev. **79** (1950), 323.
3) G. Racah, Phys. Rev. **84** (1951), 910.
4) S. P. Lloyd, Phys. Rev. **85** (1952), 904.
5) D. R. Hamilton, Phys. Rev. **74** (1948), 782; Astrophys. J. **106** (1947), 457.
6) G. Goertzel, Phys. Rev. **70** (1946), 897.
7) D. S. Ling Jr. and D. L. Falkoff, Phys. Rev. **76** (1949), 1639.
8) S. P. Lloyd, Phys. Rev. **83** (1951), 716.
9) M. E. Rose, L. C. Biedenharn and G. B. Arfken, Phys. Rev. **85** (1952), 5.
10) D. L. Falkoff and G. E. Uhlenbeck, Phys. Rev. **79** (1950), 334.
11) M. Fuchs and E. S. Lennox, Phys. Rev. **79** (1950), 221.
12) M. E. Rose and D. K. Holmes, Oak Ridge National Laboratory Report, (1951), 1022; Phys. Rev. **83** (1951), 190.
13) S. P. Lloyd, Phys. Rev. **80** (1950), 118; B. A. Lippmann, Phys. Rev. **81** (1951), 162; H. A. Tolhoek and S. R. de Groot, Phys. Rev. **83** (1951), 189.
14) E. U. Condon and G. H. Shortley, *Theory of Atomic Spectra* (Cambridge University Press, London, 1935), pp. 73–78.
15) This method is based on H. A. Bethe, Ann. d. Phys. **4** (1930), 443.
16) E. J. Konopinski and G. E. Uhlenbeck, Phys. Rev. **60** (1941), 308.
17) C. L. Longmire and A M. L. Messiah, Phys. Rev. **83** (1951), 464.
18) M. E. Rose, Phys. Rev. **51** (1937), 484.

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On the $\beta-\gamma$ Angular Correlation of Sb^{124}

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We investigate the $\beta-\gamma$ angular correlation of Sb^{124} taking into accoun the effect of the Coulomb field. It is shown that the linear combination of the three nuclear matrix elements, $\int \beta\boldsymbol{\alpha}$, $\int \beta\boldsymbol{\sigma}\times\boldsymbol{r}$ and B^3_{ij} in the first forbidden tensor interaction of the Fermi theory explains the β-decay of Sb^{124} almost completely, and in this case the transition of the nucleus is $3(-)-2(+)-0(+)$. Moreover, many other cases are discussed.

§ 1. Introduction

In the recent years, our knowledge on the β-decay has increased not only in the energy spectra but also in the angular correlations on account of the remarkable progress of the experimental technique. Especially, Sb^{124} has been investigated in both of the experiments.[1,2,3] Therefore, we study it in detail using the β-ray angular distribution functions calculated by the authors.[4]

Firstly, emitting a β-ray* Sb^{124} changes into the first excited state of Te^{124} (Te^{124*}); and secondly, emitting a γ-ray Te^{124*} changes into the ground state of Te^{124} which has spin zero and even parity presumably.

Langer, Moffat and Price[1] explained the highest energy β-ray spectrum of Sb^{124} with the a-type (first forbidden nuclear matrix elements of the Fermi theory B_{ij} or B^3_{ij}). They also decided the γ-ray as an electric dipole radiation, using the results of their measurements of the internal conversion. According to them, Sb^{124} changes as follows: Sb^{124} (spin 3, even parity) $-$ Te^{124*} (spin 1, odd parity) $-$ Te^{124} (spin 0, even parity). For brevity, we write $3(+)-1(-)-0(+)$ for this scheme hereafter.

Nakamura, Takebe and Umezawa[5] explained the β-ray spectrum with a linear combination of A^3_{ij} and T^3_{ij} terms in the second forbidden tensor interaction.

Darby and Opechowski[2] and Stevenson and Deutsch[3] measured the angular correlation coefficients of Sb^{124} (Fig. 2), and showed that $3-2-0$ and $1-1-0$ transitions with the nuclear matrix element B_{ij} (or B^3_{ij}) fit the experimental rusults comparatively well. But in these cases, both of the energy dependence and the absolute values of the angular correlation coeffieients are not sufficient; besides, in the case of $1-1-0$ other difficulty arises.**

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* The β-ray of Sb^{124} is complex and we investigate the one which has the highest maximum energy (2.29 Mev.).

** In this case the reason why the direct transition to the ground state of Te^{124} is highly forbidden is hard to be understood.

Lately Stump[6] reported that Te^{124*} has even parity and the γ–decay must occur with no change in parity according to the measurements of the polarization correlation of Sb^{124}. Metzger[7] insisted the γ–ray is unambiguously characterized by an electric quadrupole and Te^{124*} has $2(+)$, according to the measurements of the internal conversion of the γ–ray.

In Section 2 we show the possibility that a linear combination of the nuclear matrix elements can explain the β–ray spectrum and the angular correlation simultaneously. In Section 3 some other nuclear transitions are considered. In Section 4 these results are discussed and summarized.

§ 2. The linear combination of $\int \beta\alpha$, $\int \beta\sigma\times r$ and B_{ij}^{κ}

We find the linear combination of the three nuclear matrix elements, $\int i^{\beta}\alpha$, $\int i^{\beta}\sigma\times r$ and B_{ij}^{κ} in the first forbidden tensor interaction is one of the cases which give the good angular correlations of Sb^{124}. In this case, the transition scheme is $3(-)-2(+)-0(+)$.

We use Eq. (T1) of YM as the β–ray angular distribution functions. They include the effect of the Coulomb field completely. By Eq. (29) of YM the angular correlation function is

$$\begin{aligned}\mathcal{W}(\theta) =&[(5/2)a_{11}^{(0)}a_{22}'^{(0)}\{g_{11}D_{22}+d_{11}D_{22}\}+(5/2)a_{22}^{(0)}a_{22}'^{(0)}\{d_{22}G_{22}+d_{22}D_{22}+d_{22}E_{22}\}]\\&+[7a_{11}^{(2)}a_{22}'^{(2)}\{2g_{11}D_{22}-d_{11}D_{22}\}+7a_{22}^{(2)}a_{22}'^{(2)}\{2d_{22}G_{22}+d_{22}D_{22}-2d_{22}E_{22}\}\\&+(7/2)a_{12}^{(2)}a_{22}'^{(2)}d_{12}E_{22}]P_2(\cos\theta)\\&-(35/4)a_{22}^{(4)}a_{22}'^{(4)}\{6d_{22}G_{22}-4d_{22}D_{22}+d_{22}E_{22}\}P_4(\cos\theta).\end{aligned}$$

The angular distribution function of a γ quadrupole radiation is Eq. (24) of YM. The angular correlation coefficient $a(W)$ is defined by

$$a(W)=\frac{\mathcal{W}(\pi)-\mathcal{W}(\pi/2)}{\mathcal{W}(\pi/2)}.$$

We use for the nuclear radius

$$\rho=\frac{1.4\times10^{-13}A^{1/3}}{\hbar/mc},$$

and for the maximum energy of the electron

$$W_0=5.49\ mc^2.$$

In order to diminish laborious calculations, the effect of the finite nuclear size is not considered, and the approximation $\alpha ZW/p\ll1$ is used. The latter seems a considerably good approximation above the electron energy $W=4mc^2$. In the calculations of $g_{11}D_{22}$, etc., we need only their ratios. The computation is done with numerical values from the beginning, and the common factors are omitted. This is so easy that it is not necessary to construct the formulae of $g_{11}D_{22}$, etc., by rather tedious calculations.

We put

$$\frac{i\mathfrak{M}(\beta\alpha)}{\mathfrak{M}(B_{ij}^{\kappa})}=x,\quad \frac{i\mathfrak{M}(\beta\sigma\times r)}{\mathfrak{M}(B_{ij}^{\kappa})}=y,$$

where x and y are real numbers.[4] To fit the calculated angular correlation to the experimental one, we proceed as follows. At a certain electron energy W we equate the calculated angular correlation coefficient $a(W)$ to the experimental value a_{exp}. Generally, x and y which satisfy this condition form a curve of the second order. (In this case it is a ellipse.) Now, we consider at $W=5mc^2$; substituting the upper limit of the experimental value for a_{exp} $(=-0.39)$* the curve is No. 1 of Fig. 1, and substituting the lower limit of the experimental value for $a_{exp}(=-0.46)$ the curve is No. 2 of Fig. 1. The domain between the curves No. 1 and No. 2 supplies the pairs of x and y which give the good angular correlation coefficients. But this domain varies with the electron energy W, so we carry out this treatment at $W=5\,mc^2$ and $4\,mc^2$. Certain pairs of x and y which lie in the *meet* of these two domains will give the correct angular correlation.

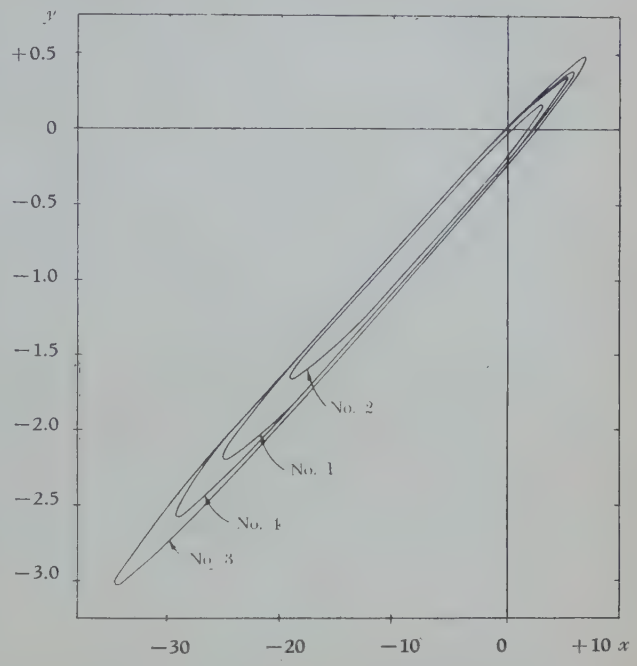

Fig. 1. Curves of the constant angular correlation coefficients for $3(-)2(+)0(+)$, $\int \beta\alpha + \int \beta\sigma\times r + B^3_{ij}$.
No. 1: $a(5)=-0{,}39$, No. 2: $a(5)=-0.46$,
No. 3: $a(4)=-0.30$, No. 4: $a(4)=-0.33$.

Moreover, we must check whether these pairs of x and y make the Kurie plots straight or not.** From Fig. 1 we choose some pairs of x and y. The angular correlation coefficients are given in Fig. 2, and the Kurie plots are given in Fig. 3. The Kurie plots are straight only above the electron energy $W=4\,mc^2$, because of the mixture of the other decay schemes below this energy. All of the chosen pairs of x and y in Fig. 2 are suitable except for B^3_{ij} only $(x=0,\ y=0)$.

In order to make the Kurie plot a straight line the correction factor must be large in the high energy region of the electron. On the contrary, in order to make the angular correlation large in this region, the sum of the parameters $a^{(0)}_{L_1L_2}$ of the angular distribution functions, which is the correction factor itself, must be small in most cases. We find $\int\beta\alpha+\int\beta\sigma\times r+B^3_{ij}$ satisfies these contradictory requirements. In this case the energy

* We use the results of Darby and Opechowski.[9]

** If we should not carry out the *trial and error* method, we must find the domain of x and y which makes the Kurie plots straight. The *meet* of this domain and the former *meet* is a favourable one. For the β-ray energy spectrum of Sb^{124} we use the results of Langer *et al*.[1]

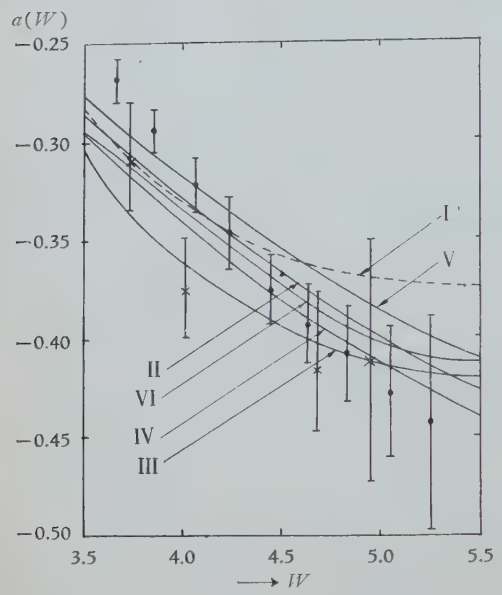

Fig. 2. The angular correlation coefficients for $3(-)-2(+)-0(+)$, $\int\beta\boldsymbol{\alpha}+\int\beta\boldsymbol{\sigma}\times\boldsymbol{r}+B^{\beta}_{ij}$.
I. $x=0$, $y=0$. II. $x=0$, $y=-0.2$.
III. $x=-5$, $y=-0.40$. IV. $x=-5$, $y=-0.63$.
V. $x=-10$, $y=-1.08$. VI. $x=-15$, $y=-1.48$.
● Experimental values of Darby and Opechowski.[2)]
× Experimental values of Stevenson and Deutsch.[3)]

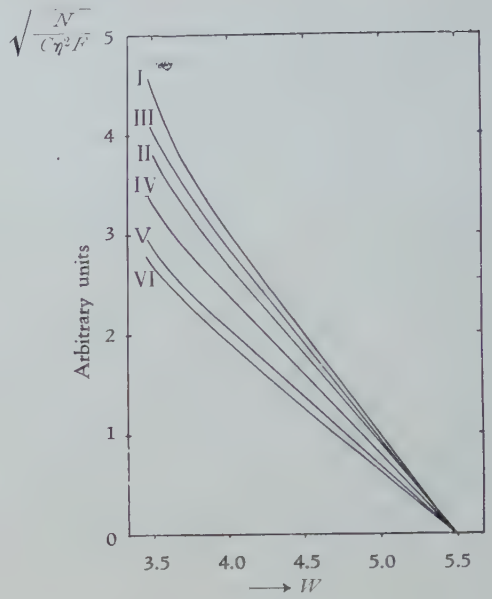

Fig. 3. The Kurie plots for $\int\beta\boldsymbol{\alpha}+\int\beta\boldsymbol{\sigma}\times\boldsymbol{r}+B^{\beta}_{ij}$.
I. $x=0$, $y=0$.
II. $x=0$, $y=-0.2$.
III. $x=-5$, $y=-0.40$.
IV. $x=-5$, $y=-0.63$.
V. $x=-10$, $y=-1.08$.
VI. $x=-15$, $y=-1.48$.

dependence of the calculated angular correlation accords with the experimental one in the limit of its error.

The *ft*-value for B^{β}_{ij} $(=(2\pi^3/G^2)\cdot\log 2/\sum|B^{\beta}_{ij}|^2)$ is of the order of $10^{10}\sim10^{11}$ (See Table I). This is considerably larger than the usual one, but it is not inconsistent with the first forbidden transition.

Table I. *ft* values for B^{β}_{ij} in the case of $\int\beta\boldsymbol{\alpha}+\int\beta\boldsymbol{\sigma}\times\boldsymbol{r}+B^{\beta}_{ij}$.

	The ratios of the nuclear matrix elements		$ft=(2\pi^3/G^2)\cdot\log 2/\sum\|B^{\beta}_{ij}\|^2$
	x	y	
I	0	0	0.28×10^{11}
II	0	−0.2	1.3×10^{11}
III	− 5	−0.40	0.32×10^{11}
IV	− 5	−0.63	1.7×10^{11}
V	−10	−1.08	2.3×10^{11}
VI	−15	−1.48	2.6×10^{11}

From these circumstances it seems that the β–decay of Sb^{124} is explained with the linear combination of $\int\beta\alpha$, $\int\beta\sigma\times r$ and B^{3}_{ij} in the first forbidden tensor interaction.

§ 3. Investigation of the other cases

We consider the other cases which differ from Section 2. We assume the following conditions at the beginning of this section.

1. The ground state of Te^{124} has spin zero and even parity.

2. The direct transition from the ground state of Sb^{124} to the ground state of Te^{124} is forbidden more highly than the one from the ground state of Sb^{124} to the first excited state of Te^{124} (Te^{124*}).

3. The case of an anomalously large nuclear matrix element (small ft value) is excluded.

These conditions are kept throughout in the following discussion. But we set up more conditions under certain circumstances, for there are too many possibilities in spite of the above conditions.

[a] Tensor interaction.

We do not use the mixture of the interaction types but only each interaction type separately. The tensor type explains the β–decay best. Therefore, we take up this type at first.

{a·1} Te^{124*} has spin two and even parity.

This is the most probable. In this case the following possibilities are found.

(a·1·1) $3(-)-2(+)-0(+)$, $\int\beta\alpha+\int\beta\sigma\times r+B^{3}_{ij}$. Discussed in Section 2.

(a·1·2) $4(-)-2(+)-0(+)$, B^{3}_{ij}. Angular correlation : bad.

(a·1·3) $4(+)-2(+)-0(+)$, $A^{3}_{ij}+T^{3}_{ij}+S^{3}_{ijk}$. This case is similar to that of Section 2. The calculation is done using Eqs. (31) and (T2) of YM. If we put

$$\frac{i\mathfrak{M}(A^{3}_{ij})}{\mathfrak{M}(S^{3}_{ijk})}=x\,,\qquad \frac{i\mathfrak{M}(T^{3}_{ij})}{\mathfrak{M}(S^{3}_{ijk})}=y\,,$$

x and y are real numbers, and the curves of the constant angular correlation coefficients are given in Fig. 4. The angular correlations and the Kurie plots are given in Figs. 5 and 6. Here we remark that the Kurie plot for S_{ijk} in Reference 1 was incorrect and the true Kurie plot is more straight than that given there. The fitness of the angular correlation and the Kurie plot is somewhat worse than that of Section 2, and moreover, a serious defect exists. Namely, the ft value for S^{3}_{ijk} $(=(2\pi^{3}/G^{2})\log 2/\sum|S^{3}_{ijk}|^{2})$ is of the order of 10^{10} (see Table II), and this is about one hundredth as large as the usual one.[8] A larger ft value may be explained by the unlikeness of the wave functions of the initial and the final states, but a smaller ft value is hard to be explained. Therefore, it seems this case is improbable.

(a·1·4) $5(+)-2(+)-0(+)$, S^{3}_{ijk}. Angular correlation : bad. ft value : too small.

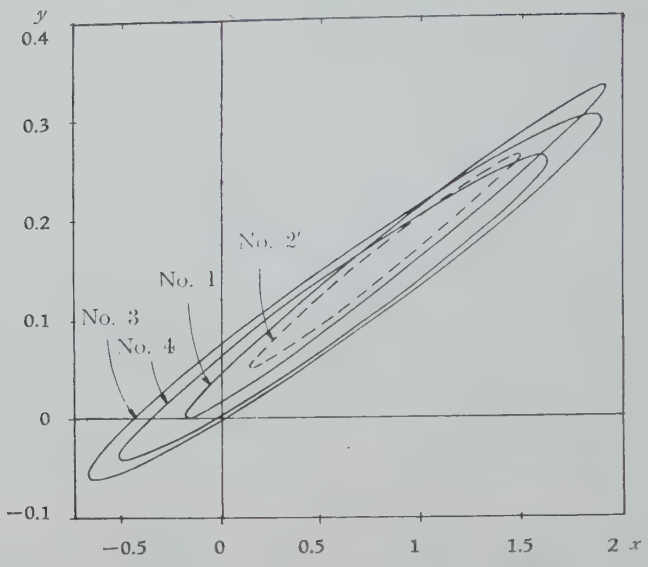

Fig. 4. Curves of the constant angular correlation coefficients for (a·1·3), 4(+)−2(+)−0(+), $A_{ij}^{\beta}+T_{ij}^{\beta}+S_{ijk}^{\beta}$.
No. 1. $a(5)=-0.39$. No. 2′. $a(5)=-0.41$.
$a(5)=-0.46$ has no solution.
No. 3. $a(4)=-0.30$. No. 4. $a(4)=-0.33$.

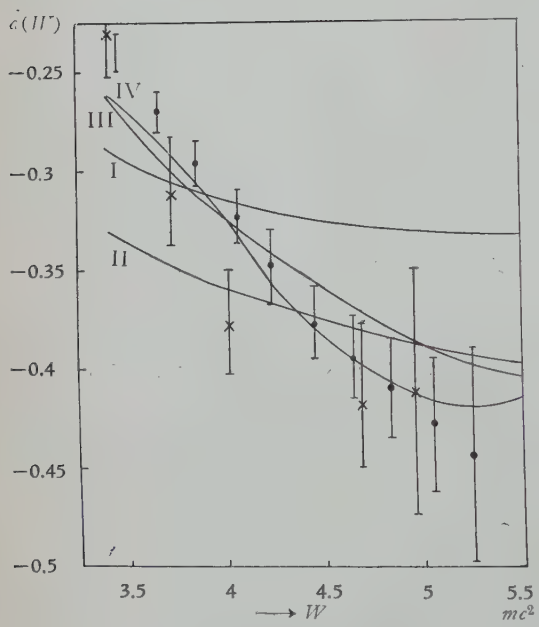

Fig. 5. The angular correlation coefficients for (a·1·3), 4(+)−2(+)−0(+), $A_{ij}^{\beta}+T_{ij}^{\beta}+S_{ijk}^{\beta}$.
I. $x=y=0$. II. $x=0.3$, $y=0.1$.
III. $x=0.8$, $y=0.18$. IV. $x=1.5$, $y=0.26$.
Cf. the note of Fig. 2.

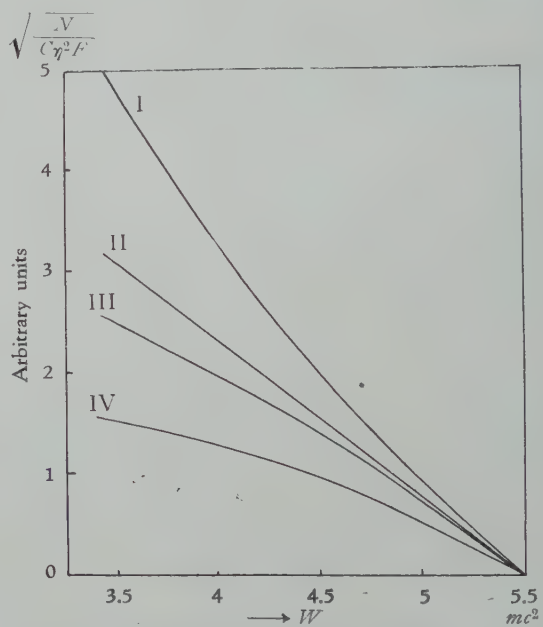

Fig. 6. The Kurie plots for (a·1·3), $A_{ij}^{\beta}+B_{ij}^{\beta}+S_{ijk}^{\beta}$.
I. $x=y=0$.
II. $x=0.3$, $y=0.1$.
III. $x=0.8$, $y=0.18$.
IV. $x=1.5$, $y=0.26$.

Table II. The ft values for S^{β}_{ijk} in the case of (a·1·3), $A^{\beta}_{ij}+T^{\beta}_{ij}+S^{\beta}_{ijk}$. $ft=(2\pi^3/G^2)\cdot\log 2/\sum|S^{\beta}_{ijk}|^2$.

	x	y	ft
I	0	0	6.3×10^9
II	0.3	0.1	1.1×10^{10}
III	0.8	0.18	1.5×10^{10}
IV	1.5	0.26	1.5×10^{10}

On the current version of the shell structure, it is not probable to assign spin five and even parity to the ground state of Sb^{124}.

{a·2} Te^{124*} has spin one and even parity.

This has been probable secondly until now.

(a·2·1) $3(-)-1(+)-0(+)$, B^{β}_{ij}. Angular correlation : bad.

(3·2·2) $4(+)-1(+)-0(+)$, S^{β}_{ijk}. Angular correlation : bad. ft value : too small.

{a·3} The other cases.

Once Langer et al[1]. thought that Te^{124*} has spin 1 and odd parity, but by the new results of Stump[6] and Metzger[7] their opinion turned out to lose its importance. We have done considerably detailed calculations in this case before the publication of the results of Stump and Metzger, so we describe the tendencies.

(a·3·1) $0(+)-1(-)-0(+)$, $\int\beta\alpha+\int\beta\sigma\times\boldsymbol{r}$. Angular correlation : very good. Kurie plot : not straight. Shell model : improbable.

(a·3·2) $2(+)-1(-)-0(+)$, $\int\beta\alpha+\int\beta\sigma\times\boldsymbol{r}+B^{\beta}_{ij}$. Angular correlation : bad. Shell modell : improbable.

(a·3·3) $3(+)-1(-)-0(+)$, B^{β}_{ij}. Angular correlation : bad.

(a·3·4) $3(-)-1(-)-0(+)$, $A^{\beta}_{ij}+T^{\beta}_{ij}+S^{\beta}_{ijk}$. Angular correlation : bad.

Whatever the ratio of the nuclear matrix elements may be, the calculated angular correlation is not so large in absolute value as the experimental one.

(a·3·5) $4(-)-1(+)-0(+)$, S^{β}_{ijk}. Angular correlation : bad. ft value : too small.

(a·3·6) Perhaps Te^{124*} has not spin two and odd parity or more than spin two, according to the measurements of the internal conversion coefficient, so that we do not consider them here.

[b] The other interaction types.

We only calculate in the cases of a single nuclear matrix element.

Generally speaking, there is no suitable case. R_{ij} and R^{β}_{ij} (spin change $3-2-0$) have a suitable angular correlation. However, the G–T type interaction exists almost certainly, so that in the case of $3-2$, parity change no, the allowed transion appears, and R_{ij} and R^{β}_{ij} are concealed.

We do not calculate for the case of the mixture of nuclear matrix elements in the

types except tensor, as it is considerably troublesome. But we expect that $\int \sigma \times r + B_{ij}$ in the first forbidden pseudovector interaction is fit to the experiments relatively well, but other cases are improbable. We do not consider the mixture of the types, for they are very complicated and we do not expect any remarkable results.

§ 4. Discussion and summary

It is difficult to explain the anomalously large $\beta-\gamma$ angular correlation of Sb^{124} by a single nuclear matrix element. If one mixes some nuclear matrix elements, whether they belong to the same interaction or not, one may be able to get the large angular correlation.

The results of Darby and Opechowski[2] and Stevenson and Deutsch[3] are somewhat different in the energy dependence. In the above sections we have used the data of Darby and Opechowski, but we can expect the same conclusions using the data of Stevenson and Deutsch.

If the β–decay is the first forbidden, the $\cos^4\theta$ term does not appear in the angular correlation function $\mathcal{W}(\theta)$; on the contrary, if the β–decay is the second forbidden and the γ–ray is not a dipole, the $\cos^4\theta$ term appears generally. This term may be small, but if it will be distinguished we shall be able to exclude the first forbidden transition.

The main tendency of the angular correlation with a single nuclear matrix element will not be determined by the nuclear matrix elements but by the spin change and the rank of the interaction Hamiltonian. But one cannot generalize the above conclusion in the case of the mixture of more than two nuclear matrix elements. The effect of these interaction terms has large influence.

In conclusion, the large angular correlation of Sb^{124} does not contradict the Fermi theory and it can be explained with the linear combination of the three nuclear matrix elements, $\int \beta\alpha$, $\int \beta\sigma \times r$ and B_{ij}^3 in the first forbidden tensor interaction. The transition $3(-)-2(+)-0(+)$ of the nucleus is almost certain.

The authors wish to express their sincere thanks to Professor S. Nakamura and to Mr. M. Umezawa for their continuous guidance and encouragement and to Professor T. Miyazima for the suggestion of this problem. They are also grateful to Mr. H. Taneichi for his kind assistance. They are indebted to the "Yukawa Yomiuri Fellowship" for the financial aid.

References

1) L. M. Langer, R. D. Moffat and H. C. Price Jr. Phys. Rev. **79** (1950), 808 ; L. M. Langer, Phys. Rev. **84** (1951), 1059.
2) E. K. Darby and W. Opechowski, Phys. Rev. **83** (1951), 676, and private communication to Professor S. Nakamura.
3) D. T. Stevenson and M. Deutsch, Phys. Rev. **83** (1951), 1202.
4) M. Yamada and M. Morita, Prog. Theor. Phys. **8** (1952), 431. Called YM hereafter.
5) S. Nakamura, H. Takebe and M. Umezawa, Prog. Theor. Phys. **6** (1951), 604 ; Phys. Rev. **83** (1951), 1273.
6) R. Stump, Phys. Rev. **86** (1952), 249.
7) F. R. Metzger, Phys. Rev. **86** (1952), 435.
8) M. G. Mayer, S. A. Moszkowski and L. W. Nordheim, Rev. Mod. Phys. **23** (1951), 315.

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On the Determination of the Elastic Spectra of Solids from Specific Heat Data

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A new method is proposed which allows to express the frequency-distribution-function of solids by real functions. The result can be written in such a way that it contains the experimental data in terms of a modified Debye-temperature.

§ 1. Introduction

The problem to find the elastic spectra of solids from the specific heat has recently received much interest. Montroll[1] has solved the problem by the method of Fourier-transforms. This solution involves complex functions which make a direct application to actual problems impossible. Grayson-Smith and Stanley[2] have solved the integral equation in question by expanding the frequency-distribution into a Fourier-series. This method is appropriate only when low-temperature data of the specific heat are used.

We intend to find an expression for the frequency-distribution in terms of real functions and we propose the following way.

§ 2. Method

We write the number of eigen-vibrations of the solid in the frequency-interval between ν and $\nu+d\nu$ as $f(\nu/\nu_0)\,d\nu/\nu_0$, where ν_0 is a frequency in unit of which we express the frequencies. Its value we choose in a way explained later. The specific heat per mode $C(T)$ at the temperature T is then written as

$$C(T)=\frac{k}{\nu_0}\int_0^\infty d\nu\,\frac{(h\nu/kT)^2 f(\nu/\nu_0)}{(e^{h\nu/kT}-1)(1-e^{-h\nu/kT})}\,.$$

Introducing $x\equiv kT/h\nu_0$ and $z\equiv h\nu/kT$, we obtain with $f(z)\equiv z^2 g(z)$ and $C(x)\equiv kx^3F(x)$

$$F(x)=\int_0^\infty dz\,\frac{z^4 g(xz)}{(e^z-1)(1-e^{-z})}\,. \qquad (1)$$

Our problem to determine the frequency-distribution $g(z)$ by means of the specific heat $F(x)$ is now to solve this integral equation (1) of $g(z)$. Using the Fourier-integral of $F(x)$

$$F(x) \equiv \frac{2}{\pi} \int_0^\infty dt\, \varphi(t) \cos xt\,, \quad \varphi(t) = \int_0^\infty du\, F(u) \cos tu\,, \tag{2, 2a}$$

we express $g(z)$ by the integral

$$g(z) \equiv \frac{2}{\pi} \int_0^\infty dt\, \varphi(t) \gamma(zt)\,, \tag{3}$$

$$= \frac{2}{\pi} \int_0^\infty dt\, \gamma(zt) \int_0^\infty du\, F(u) \cos tu\,, \tag{3a}$$

where $\gamma(z)$ has to satisfy the following equation obtained by insertion of eqs. (2) and (3) into eq. (1)

$$\cos x = \int_0^\infty dz\, \frac{z^4 \gamma(xz)}{(e^z - 1)(1 - e^{-z})}\,. \tag{4}$$

If we could find the solution of this integral equation (4) in real functions then eq. (3a) would be a form satisfying our intention.

In order to solve eq. (4) we observe that the homogeneous equation:

$$\psi(x) = \lambda \int_0^\infty dz \frac{z^4 \psi(xz)}{(e^z - 1)(1 - e^{-z})} \tag{5}$$

has the solutions $\psi(x) = x^\alpha$ where α can take any value for which the integral has a meaning. Since $\cos x$ can be expanded into a power series, we are allowed to assume that $\gamma(z)$ can also be expanded into a power series and find then easily

$$\gamma(z) = \sum_{\nu=0}^\infty (-)^\nu \frac{z^{2\nu}}{(2\nu)!\,(2\nu+4)!\,\zeta(2\nu+2)}\,, \tag{6}$$

$\zeta(x)$ being the Riemann ζ–function. With the relations

$$\sum_{\nu=0}^\infty (-)^\nu \frac{x^{2\nu}}{(2\nu)!\,(2\nu+4)!} = \mathrm{Re}\left[\frac{J_4(2\sqrt{ix})}{ix^2}\right] \tag{7}$$

and

$$\frac{1}{\zeta(x)} = \sum_{n=1}^\infty \frac{\mu(n)}{n^x}\,, \tag{8}$$

$\mu(n)$ being the Moebius function, eq. (6) takes the form aimed by us as follows.

$$\gamma(z) = \sum_{n=1}^\infty \frac{\mu(n)}{n^2} \mathrm{Re}\left[\frac{J_4(2\sqrt{iz/n})}{i(z/n)^2}\right]. \tag{9}$$

To get further, we express the temperature dependence of the specific heat, $F(x)$, in terms of a modified Debye-temperature $\vartheta(x)$ as

$$F(x) \equiv 3 \int_0^{\vartheta(x)/x} dz\, \frac{z^4}{(e^z - 1)(1 - e^{-z})}\,. \tag{10}$$

Now we come to a definition of the frequency ν_0. It seems convenient to choose ν_0 in such a way that $h\nu_0/k$ is the minimum Debye-temperature of the solid in question. With this expression eq. (10) for $F(x)$, we rewrite eq. (2a)

$$\varphi(t)=3\int_0^{\infty} du\cos tu\int_0^{\vartheta(u)/u} dz\frac{z^3}{(e^z-1)(1-e^{-z})}. \tag{11}$$

By a partial integration and a change of the integration variable u into v

$$\vartheta(u)/u\equiv v \quad \text{or} \quad u\equiv\chi(v), \tag{12}$$

χ being the inversion of the definition of v, we obtain

$$\varphi(t)=\frac{3}{t}\int_0^{\infty} dv\sin(t\chi(v))\frac{v^4}{(e^v-1)(1-e^{-v})}, \tag{13}$$

the insertion of which into eq. (3) gives our final result

$$g(z)=3\frac{2}{\pi}\int_0^{\infty} dt\frac{\sin t}{t}\int_0^{\infty} dv\frac{v^4\gamma(zt/\chi(v))}{(e^v-1)(1-e^{-v})}. \tag{14}$$

Especially, in the Debye case, $\vartheta(x)$ has the constant value unity and $\chi(v)=1/v$. Then with eq. (4) we find

$$g(z)=3\frac{2}{\pi}\int_0^{\infty} dt\frac{\sin t\cos zt}{t}=\begin{cases}3 : 0\leq z\leq 1,\\ 0 : z>1,\end{cases} \tag{15}$$

which leads to the well known Debye frequency-distribution

$$\frac{1}{\nu_0}f\left(\frac{\nu}{\nu_0}\right)=\begin{cases}3\nu^2/\nu_0^3 : 0\leq\nu\leq\nu_0,\\ 0 : \nu>\nu_0,\end{cases} \tag{16}$$

as it must be.

A discussion of our results we reserve for another publication.

Appendix

It may be of interest here to see that the integral-expression of $g(z)$, eq. (3), is allowable. We observe that $g(z)$ can obviously be expressed as a Fourier-integral

$$g(z)=\frac{2}{\pi}\int_0^{\infty} dt\cos zt\int_0^{\infty} du\cos tu\cdot g(u).$$

Applying for $\cos zt$ eq. (4)

$$g(z)=\frac{2}{\pi}\int_0^{\infty} dt\int_0^{\infty} dv\frac{v^4\gamma(ztv)}{(e^v-1)(1-e^{-v})}\int_0^{\infty} du\cos tu\cdot g(u),$$

$$=\frac{2}{\pi}\int_0^{\infty} dt\,\gamma(zt)\int_0^{\infty} du\cos tu\int_0^{\infty} dv\frac{v^4 g(uv)}{(e^v-1)(1-e^{-v})},$$

$$= \frac{2}{\pi} \int_0^\infty dt\, \gamma(zt) \int_0^\infty du\, F(u) \cos tu\,,$$

$$= \frac{2}{\pi} \int_0^\infty dt\, \varphi(t)\, \gamma(zt)\,.$$

References

1) E. W. Montroll, J. Chem. Phys. **10** (1942), 218 and **11** (1943), 481.
2) H. Grayson-Smith and J. P. Stanley, J. Chem. Phys. **18** (1950), 236.

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A Statistical Theory of Linear Dissipative Systems*

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On the basis of the joint probability for the two states occurring at different times proposed by Onsager, the theory of Brownian motion is generalized to the case of isolated systems such as treated by "the thermodynamics of irreversible processes." Fokker-Planck's and Langevin's equations are also generalized. When the deviations from thermal equilibrium are so small that the entropy of the system is expressible in a quadratic form with respect to its state variables, these equations are integrated, and the probability distribution for the state variables at each time is obtained.

As two examples, the problems of the Brownian motion of a free colloidal particle in a uniform isotropic medium and of the heat conduction along an isolated one-dimensional rod are treated. The result of the former coinsides with the usual one, but that of the latter differs essentially from the Orstein-Milatz theory.

§ 1. Introduction

Many attempts to build up "the thermodynamics of irreversible processes" by making use of Onsager's reciprocal relations have recently been accomplished with a certain success[1]. The next fundamental problem to be solved is of course to seek for the molecular theoretical generalization of this new thermodynamics, especially its relation to statistical mechanics. Before these researches, however, it seems to be necessary, as a preliminary, to examine its relation to the old theories of fluctuation phenomena given by Einstein, Smoluchowski, Fürth, and others[2]. We shall do this preliminary work in this article.

In order to avoid physical ambiguities, let us consider mainly *isolated systems*, each macroscopic state of which is assumed to be specified by a set of values α_1', α_2', $\cdots$, α_N' of *macroscopic variables* α_1, α_2, $\cdots$, α_N; e.g. a set of temperatures of the small parts of the system (cf., § 5). According to the thermodynamics of *non-uniform* systems, a value of entropy $S(\alpha')$ is supposed to correspond to each state α' of the system, provided that every small part of the system is substantially in its thermal equilibrium state. Assuming the *quasi-static process* in its extended sense, the rate of change of entropy is given by

$$\frac{dS(\alpha')}{dt}=\frac{1}{T^0}\sum_{i=1}^{N}A_i(\alpha')\frac{d\alpha_i'}{dt}, \tag{1·1}$$

* The main idea of this article (§§ 1, 2, and 4) was already reported in Japanese: Bussei-ron Kenkyu, (Mimeographed Circular in Japanese) No. 45 (1951), 63; No. 46 (1952), 92.

where T^0 denotes the temperature of the system at thermal equilibrium, and $A(\alpha')$ the affinity defined by

$$A_i(\alpha') \equiv T^0 \frac{\partial S(\alpha')}{\partial \alpha_i'}. \tag{1·2}$$

Since the rate of change (1·1) must be equal to the rate of irreversible production of entropy $(dS/dt)_{irr.}$ because of isolation of the system, we shall assume here, in "the thermodynamics of irreversible processes", the phenomenological *linear relations*

$$\frac{d\alpha_i'}{dt} = \sum_{j=1}^{N} L_{ij} A_j(\alpha'), \tag{1·3}$$

and *Onsager's reciprocal relations* between the kinetic coefficients

$$L_{ij} = L_{ji}\ ^{*)}. \tag{1·4}$$

When the assumption (1·3) is permissible, we shall call the system to be *linear dissipative*. The second law of thermodynamics imposes the conditions for the matrix (L_{ij}) to be positive definite.

At this point Onsager[3] found the fact that Eq. (1·3), which determines the course of an irreversible process, can be derived from the variation principle, *the principle of the least dissipation of energy*

$$\frac{dS}{dt} - \frac{\Phi}{T^0} = \max., \tag{1·5}$$

under the assumption of Eq. (1·4). Here Φ denotes the dissipation function

$$\Phi \equiv \frac{1}{2} \sum_{i,j=1}^{N} R_{ij} \frac{d\alpha_i'}{dt} \frac{d\alpha_j'}{dt}, \tag{1·6}$$

the matrix (R_{ij}) being the reciprocal of (L_{ij}):

$$\left.\begin{aligned} \sum_{l=1}^{N} L_{il} R_{lj} = \sum_{l=1}^{N} R_{il} L_{lj} = \delta_{ij}, \\ R_{ij} = R_{ji}. \end{aligned}\right\} \tag{1·7}$$

Further, he compared Eq. (1·5) with the variation principle determining the equilibrium state α^0:

$$S = \max., \tag{1·8}$$

taking *Boltzmann's principle*

$$k \log W(\alpha') = S(\alpha') + \text{const.} \tag{1·9}$$

into account, and proposed, as a statistical interpretation of Eq. (1·5), the *joint* probability $W(\alpha', \Delta t, \alpha'')$ for the two states α' and $\alpha'' \equiv \alpha' + \Delta\alpha'$ occurring at the times t and $t' \equiv t + \Delta t$ respectively:

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* For the sake of simplicity we confine ourselves to the case of no magnetic field, or no Coriolis force (cf. Casimir[4]).

$$k \log W(\alpha', \Delta t, \alpha'') = \frac{1}{2}\left\{S(\alpha') + S(\alpha'') - \frac{\Phi(\Delta\alpha', \Delta\alpha')}{T^0 \Delta t}\right\} + \text{const.},^* \qquad (1\cdot10)$$

where

$$\Phi(\Delta\alpha', \Delta\alpha') \equiv \frac{1}{2}\sum_{i,j=1}^{N} R_{ij}\,\Delta\alpha_i'\,\Delta\alpha_j'. \qquad (1\cdot11)$$

k denotes Boltzmann's constant, the parameter that is in close connection with fluctuations.

The probability (1·10) gives in fact Eq. (1·3) as the one representing the most probable course of the irreversible process. This will more easily be seen by introducing the transition probability from the state α' to the state α'':

$$\Psi(\alpha', \Delta t, \alpha'') = W(\alpha', \Delta t, \alpha'')/W(\alpha'), \qquad (1\cdot12)$$

as we shall show in the next section. On the other hand, if we find the concrete expression for the transition probability, we shall at once be able to construct a statistical theory of irreversible processes on the model of Brownian motion theories, and this construction is our principal aim in this article. Thus, in conformity with its general importance we shall call Eq. (1·10) *Onsager's principle*.

§ 2. General theory

In this section we shall first derive the approximate expression for the transition probability $\Psi(\alpha', \Delta t, \alpha'')$, and, making use of this, obtain Fokker-Planck's equation. Next we shall introduce the fluctuating part of the affinity, by which we shall generalize Langevin's equation in the theory of Brownian motion.

From Eqs. (1·12), (1·10), and (1·9) we obtain

$$k \log \Psi(\alpha', \Delta t, \alpha'') = \frac{1}{2}\left\{\Delta S - \frac{\Phi(\Delta\alpha', \Delta\alpha')}{T^0 \Delta t}\right\} + \text{const.}, \qquad (2\cdot1)$$

where

$$\Delta S \equiv S(\alpha'') - S(\alpha') = (\Delta S)_{irr.} \qquad (2\cdot2)$$

If we notice $\Delta\alpha' = O(\Delta t)$ and

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* The reason why the factor 1/2 was inserted is as follows: From Eq. (2·6) we have

$$\langle a_i(t')a_j(t')\rangle_{\alpha(t)=\alpha'} + a_i'a_j' - a_i'\langle a_j(t')\rangle_{\alpha(t)=\alpha'} - \langle a_i(t')\rangle_{\alpha(t)=\alpha'}a_j' = 2kT^0 L_{ij}\Delta t,$$

or, averaging this over all possible values of α' with the weight $W(\alpha')$,

$$\langle\langle a_i(t')a_j(t')\rangle\rangle + \langle a_i(t)a_j(t)\rangle - \langle\langle a_i(t)a_j(t')\rangle\rangle - \langle\langle a_i(t')a_j(t)\rangle\rangle = 2kT^0 L_{ij}\Delta t.$$

On the other hand, by the temporal homogeneity and of the microscopic reversibility:

$$\langle\langle a_i(t')a_j(t')\rangle\rangle = \langle a_i(t)a_j(t)\rangle \equiv A_{ij}(0),$$

$$\langle\langle a_i(t)a_j(t')\rangle\rangle = \langle\langle a_i(t')a_j(t)\rangle\rangle \equiv A_{ij}(\Delta t),$$

we obtain $$A_{ij}(\Delta t) = A_{ij}(0) - kT^0 L_{ij}\Delta t,$$

which is nothing less than the Onsager's (4·7) in his second paper[3], if we put $T^0 L_{ij} \equiv G_{ij}$.

$$\Delta S=\frac{1}{T^0}\sum_{i=1}^{N}A_i(\alpha')\Delta\alpha_i'+O(\Delta t^2), \tag{2·3}$$

we may rewrite Eq. (2·1) into the form

$$\Psi(\alpha',\ \Delta t,\ \alpha'')=N(\alpha')\exp\Big[-\sum_{i,j=1}^{N}\frac{R_{ij}}{4kT^0\Delta t}\Big\{\Delta\alpha_i'-\sum_{l=1}^{N}L_{il}A_l(\alpha')\Delta t\Big\}$$

$$\cdot\Big\{\Delta\alpha_j'-\sum_{m=1}^{N}L_{jm}A_m(\alpha')\Delta t\Big\}+O(\Delta t^2)\Big], \tag{2·4}$$

where $N(\alpha')$ is a normalization factor. The expression (2·4) gives a distribution for the amount of change $\Delta\alpha'$ occurring from the *fixed* initial state α' during the small time Δt. The first two moments of this distribution are as follows:

$$\langle\Delta\alpha_i\rangle_{\alpha(t)=\alpha'}=\sum_{j=1}^{N}L_{ij}A_j(\alpha')\Delta t+O(\Delta t^2), \tag{2·5}$$

$$\langle\Delta\alpha_i\Delta\alpha_j\rangle_{\alpha(t)=\alpha'}=2kT^0L_{ij}\Delta t+O(\Delta t^2). \tag{2·6}$$

At a glance it will be seen that the most probable course determined by Eq. (2·5) agrees with the one determined by Eq. (1·3)[3)4)].

In order to obtain Fokker-Planck's equation we must assume the stochastic process under consideration to be Markoffian, i.e., the validity of Smoluchowski's equation in the form:

$$W(\alpha',\ t+\Delta t)=\int\cdots\int W(\alpha'-\Delta\alpha',\ t)\Psi(\alpha'-\Delta\alpha',\ \Delta t,\ \alpha')\prod_{i=1}^{N}d(\Delta\alpha_i'), \tag{2·7}$$

where the integration should be taken over all possible values of $\Delta\alpha_i$. For a sufficiently small Δt the transition probability (2·4) will have the form of sharp Gaussian distribution, so that the integration range may be replaced approximately by $(-\infty,\ \infty)$. Making use of Eqs. (2·5) and (2·6), we obtain by the usual procedure[5)]

$$\frac{\partial W(\alpha',\ t)}{\partial t}=\sum_{i,j=1}^{N}\frac{\partial}{\partial\alpha_i'}\Big[D_{ij}\Big\{\frac{\partial W(\alpha',\ t)}{\partial\alpha_j'}-\frac{A_j(\alpha')}{kT^0}W(\alpha',\ t)\Big\}\Big], \tag{2·8}$$

where

$$D_{ij}\equiv kT^0L_{ij}=kT^0(R^{-1})_{ij}. \tag{2·9}$$

It will be interesting to notice that the affinity $A(\alpha')$ plays again the role of driving force as in Eq. (1·3), and that the generalized diffusion constant D is given by the generalized *Einstein relation* (2·9), since R has formally the meaning of resistance. The fundamental solution $W(\alpha',\ t)$, which satisfies the initial condition of the type

$$W(\alpha',\ 0)=\prod_{i=1}^{N}\delta(\alpha_i'-\alpha_i^*), \tag{2·10}$$

determines the probability that given α^* we find α in the range $(\alpha',\ \alpha'+d(\Delta\alpha'))$ a *finite* time t later. In the limit $t\to\infty$ it must converge therefore to the equilibrium distribution $W(\alpha')$ given by Eq. (1·9). In fact we see that $W(\alpha')$ is only one stationary solution of Eq. (2·8) because of the definition of the affinity (1·2).

We have shown above that the linear relation (1·3) is valid on the average*. Now we shall generalize it into a *stochastic differential equation*, which will be valid without averaging procedure:

$$\frac{du_i}{dt}=\sum_{j=1}^{N} L_{ij}\{A_j(a)+\mathcal{A}_j(a,t)\} \tag{2·11}$$

by introducing a fluctuating part of the affinity $\mathcal{A}(a,t)$. Since a becomes a random variable, the systematic part of the affinity $A(a)$ should also be regarded as a random function, the functional form of which is the same as that defined by Eq. (1·2). The statistical property of $\mathcal{A}(a,t)$ is supposed to be determined by Onsager's principle. Integrating Eq. (2·11) with the initial condition $a(t)=a'$, we have

$$\Delta a_i=\sum_{j=1}^{N} L_{ij}\{A_j(a')\,\Delta t+B_j(a',\Delta t)\}\;; \tag{2·12}$$

$$B_j(a',\Delta t)\equiv\int_t^{t+\Delta t}\mathcal{A}_j(a',\xi)\,d\xi, \tag{2·13}$$

for a time interval of duration Δt large compared with the average period of a single fluctuation of $\mathcal{A}(a,\xi)$ but small enough for the change Δa to be negligible in the arguments of $A(a)$ and $\mathcal{A}(a,\xi)$. The probability distribution for the random variable $B(a',\Delta t)$ is obtained from Eq. (2·4):

$$\Psi(a',\Delta t,a'')=N(a')\exp\left[-\sum_{i,j=1}^{N}\frac{L_{ij}}{4kT^0\Delta t}B_i'(a',\Delta t)B_j'(a',\Delta t)\right], \tag{2·14}$$

the terms $O(\Delta t^2)$ being neglected. B' denotes a special value of B. Similarly the first two moments are given by

$$\langle B_i(a',\Delta t)\rangle_{a(t)=a'}=0, \tag{2·15}$$

$$\langle B_i(a',\Delta t)B_j(a',\Delta t)\rangle_{a(t)=a'}=2kT^0R_{ij}\Delta t. \tag{2·16}$$

Since the higher moments have no physical importance because of the special construction of the dissipation function itself, (1·11) or (1·6), the preceding results exhaust the statistical knowledge given by Onsager's principle. Thus the validity of Onsager's principle (1·10) will be justified by the experimental justification of Eqs. (2·15) and (2·16).

For linear dissipative systems the validity of Eq. (2·15) may be considered as being justified by the empirical linear law (1·3), while the experimental basis for Eq. (2·16) has to be seeked for in the observations of fluctuation phenomena, e.g., fluctuations in temperature, concentrations, electric current, and so on. For this purpose it is more convenient to rewrite Eqs. (2·15) and (2·16) into more usual forms by imposing on the properties of $\mathcal{A}(a,\xi)$ a few plausible conditions. These conditions will, however, be inevitably of somewhat rough character. Let us first treat Eq. (2·15). Remembering the definition (2·13), and interchanging the order of integrations, we shall have

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* In the case of diffusion, Sugita[1] already pointed out that Eq. (1·3) corresponds to averaged Langevin's equation.

$$\langle B_i(\alpha', \Delta t)\rangle_{\alpha(t)=\alpha'} = \int_t^{t+\Delta t} \langle \mathcal{A}_i(\alpha', \xi)\rangle_{\alpha'} d\xi = 0, \tag{2·17}$$

where the symbol $\langle\cdots\rangle_{\alpha'}$ represents some averages that may contain partly the time average over the interval $(t, t+\Delta t)$. If the ietegrand $\langle \mathcal{A}_i(\alpha', \xi)\rangle_{\alpha'}$ does not vary with ξ, we obtain

$$\langle \mathcal{A}_i(\alpha', \xi)\rangle_{\alpha'} = 0. \tag{2·18}$$

In the similar manner, Eq. (2·16) becomes

$$\begin{aligned}\langle B_i(\alpha', \Delta t) B_j(\alpha', \Delta t)\rangle_{\alpha(t)=\alpha'} &= \iint_t^{t+\Delta t} \langle \mathcal{A}_i(\alpha', \xi)\mathcal{A}_j(\alpha', \xi')\rangle_{\alpha'} d\xi\, d\xi' \\ &= 2kT^0 R_{ij}\Delta t,\end{aligned} \tag{2·19}$$

or

$$\int_{-\infty}^{+\infty} \langle \mathcal{A}_i(\alpha', \xi)\mathcal{A}_j(\alpha', \xi+\tau)\rangle_{\alpha'}\, d\tau = 2kT^0 R_{ij} \tag{2·20}$$

approximately, if the integrand $\langle \mathcal{A}_i(\alpha', \xi)\mathcal{A}_j(\alpha', \xi+\tau)\rangle_{\alpha'}$ is independent of ξ and vanishes very rapidly with increasing $|\tau|$. Since the kinetic coefficient L in Eq. (1·3), and hence its reciprocal R, is assumed to be constant, the apparent dependence of the integrand $\langle \mathcal{A}_i(\alpha', \xi)\mathcal{A}_j(\alpha', \xi+\tau)\rangle_{\alpha'}$ on α' is effectively compensated by integration. Now let us examine experimental justification of Eq. (2·20). This must of course be done in each case, but the general validity of Eq. (2·20) will be made plausible by the following consideration. In the case of electric current there are the well-known Johnson's experiment and its Nyquist's theory[6]. After some generalizations, *Nyquist's equation* may be written in the form

$$\langle \mathcal{A}_i(\alpha', \xi)\mathcal{A}_j(\alpha', \xi+\tau)\rangle_{\alpha'} = 2kT^0 R_{ij}\delta(\tau), \tag{2·21}$$

where $\delta(\tau)$ denotes Dirac's delta function. The relation (2·21) satisfies Eq. (2·20). Thus the general validity of Onsager's principle (1·10) may be considered as made plausible.

In the preceding paragraphs we have shown that Onsager's principle describes any irreversible process of linear dissipative systems including fluctuations, and that the fluctuation is closely connected, through the kinetic coefficients, with the energy dissipation as in the original idea of Nyquist[6]. The latter fact was the reason why we have coupled $A(\alpha)$ and $\mathcal{A}(\alpha, t)$ in Eq. (2·11). From the former fact we see that Onsager's principle plays the role of the second law of thermodynamics. If we take into account that our theory is, from its beginning, closely related with the well-known method of Boltzmann in statistical mechanics, it will be seen that Onsager's principle gives an expression for the famous statistical interpretation of the second law of thermodynamics by Boltzmann. By this interpretation the entropy of an isolated system may increase as well as decrease, though it must increase on the average. In our theory this temporal behaviour of entropy will be most explicitly described by the *stochastic* differential equation

$$\frac{dS(a)}{dt}=\frac{1}{T^0}\sum_{i=1}^{N}A_i(a)\frac{da_i}{dt} \tag{2·22}$$

$$=\frac{1}{T^0}\sum_{i,j=1}^{N}L_{ij}A_i(a)\{A_j(a)+\mathcal{A}_j(a,t)\}$$

$$=\left(\frac{dS}{dt}\right)_{irr.}(a)+\mathcal{S}(a,t), \tag{2·23}$$

where

$$\mathcal{S}(a,t)\equiv\frac{1}{T^0}\sum_{i,j=1}^{N}L_{ij}A_i(a)\mathcal{A}_j(a,t); \tag{2·24}$$

$$\langle\mathcal{S}(a',\xi)\rangle_{a'}=0, \tag{2·25}$$

$$\int_{-\infty}^{+\infty}\langle\mathcal{S}(a',\xi)\mathcal{S}(a',\xi+\tau)\rangle_{a'}d\tau=2k\left(\frac{dS}{dt}\right)_{irr.}(a'). \tag{2·26}$$

[the use of the reciprocal relations (1·4) being made]. Since the first term of Eq. (2·23) is a positive definit quadratic form, the entropy will increase on the average, except for at the equilibrium state a^0 defined by Eq. (1·8), i.e. by

$$A_i(a^0)=T^0\frac{\partial S(a^0)}{\partial a_i{}^0}=0. \tag{2·27}$$

§ 3. Special case of a quadratic entropy

In this section we shall confine ourselves to the case of sufficiently small deviations $a'-a^\circ$ from the equilibrium state a°, so that the assumption of independence of the fluctuations on a' may be permissible. In this case the entropy for a state a' is given in a sufficient approximation by

$$S(a')=S^0-\frac{1}{2}\sum_{i,j=1}^{N}S_{ij}(a_i'-a_i{}^0)(a_j'-a_j{}^0); \tag{3·1}$$

$$S_{ij}=S_{ji}\left[\equiv-\frac{\partial^2S(a^0)}{\partial a_i{}^0\partial a_j{}^0}\right]. \tag{3·2}$$

The matrix (S_{ij}) should be positive definite by virtue of the second law of thermodynamics. The affinity (1·2) has the form

$$A_i(a')=-T^0\sum_{j=1}^{N}S_{ij}(a_j'-a_j{}^0), \tag{3·3}$$

which gives in turn the frictional force

$$\sum_{j=1}^{N}L_{ij}A_j(a')=-\sum_{j=1}^{N}\Lambda_{ij}(a_j'-a_j{}^0), \tag{3·4}$$

where

$$\Lambda_{ij}\equiv T^0\sum_{l=1}^{N}L_{il}S_{lj}=\frac{1}{k}\sum_{l=1}^{N}D_{il}S_{lj}. \tag{3·5}$$

Though the matrices (L_{ij}) and (S_{ij}) are symmetric, the matrix (Λ_{ij}) is not so in general. In the following we shall see that this matrix (Λ_{ij}) will determine the relaxation time spectrum of the process under consideration.

Fokker-Planck's equation (2·8) has the form

$$\frac{\partial W(a', t)}{\partial t} = \sum_{i=1}^{N} \frac{\partial}{\partial (a_i' - a_i^0)} \left\{ \sum_{j=1}^{N} \Lambda_{ij} (a_j' - a_j^0)\, W(a', t) \right\}$$

$$+ \sum_{i,j=1}^{N} D_{ij} \frac{\partial^2 W(a', t)}{\partial (a_i' - a_i^0)\, \partial (a_j' - a_j^0)}. \tag{3·6}$$

This equation can be solved by the orthogonal transformation[7]

$$\eta_\tau = \sum_{i=1}^{N} \psi_{\tau i} (a_i - a_i^0), \tag{3·7}$$

where the coefficients $\psi_{\tau i}$ are determined by the eigenvalue problem

$$\sum_{i=1}^{N} \psi_{\tau i} \Lambda_{ij} = \lambda_\tau \psi_{\tau j}, \tag{3·8}$$

λ_τ being an eigenvalue. By this transformation Eq. (3·6) becomes

$$\frac{\partial W(\eta', t)}{\partial t} = \sum_{\tau} \lambda_\tau \frac{\partial}{\partial \eta_\tau'} \{ \eta_\tau' W(\eta', t) \} + \frac{1}{2} \sum_{\tau,\epsilon} \sigma_{\tau\epsilon} \frac{\partial^2 W(\eta', t)}{\partial \eta_\tau' \partial \eta_\epsilon'}, \tag{3·9}$$

where we have defined

$$\sigma_{\tau\epsilon} \equiv 2 \sum_{i,j=1}^{N} \psi_{\tau i} D_{ij} \psi_{\epsilon j}. \tag{3·10}$$

The fundamental solution, which satisfies the initial condition

$$W(\eta', 0) = \prod_{\tau} \delta(\eta_\tau' - \eta_\tau^*), \tag{3·11}$$

is given by

$$W(\eta', t) = N(t) \exp\left[-\frac{1}{2} \sum_{\tau,\epsilon} \Gamma_{\tau\epsilon} (\eta_\tau' - \eta_\tau^* e^{-\lambda_\tau t}) (\eta_\epsilon' - \eta_\epsilon^* e^{-\lambda_\epsilon t}) \right], \tag{3·12}$$

where $N(t)$ denotes the normalization factor, and

$$(\Gamma^{-1})_{\tau\epsilon} \equiv \frac{\sigma_{\tau\epsilon}}{\lambda_\tau + \lambda_\epsilon} [1 - \exp\{-(\lambda_\tau + \lambda_\epsilon) t\}]. \tag{3·13}$$

The corresponding solution of Eq. (3·6) will be obtained by making use of the inverse transformation of Eq. (3·7). This will be carried out easily when the matrix (S_{ij}) is diagonal.

The stochastic differential equation (2·11) has the form

$$\frac{d(a_i - a_i^0)}{dt} = -\sum_{j=1}^{N} \Lambda_{ij} (a_j - a_j^0) + \mathcal{F}_i(t), \tag{3·14}$$

where we have neglected the dependence of the fluctuating term on α, and defined

$$\mathcal{F}_i(t) \equiv \sum_{j=1}^{N} L_{ij}\, \mathcal{A}_j(t). \tag{3·15}$$

The statistical properties of $\mathcal{F}$ are determined by Eqs. (2·18) and (2·20) :

$$\langle \mathcal{F}_i(\xi) \rangle_{\alpha'} = 0, \tag{3·16}$$

$$\int_{-\infty}^{+\infty} \langle \mathcal{F}_i(\xi) \mathcal{F}_j(\xi+\tau) \rangle_{\alpha'} d\tau = 2D_{ij}. \tag{3·17}$$

After the transformation (3·7), Eq. (3·14) becomes

$$\frac{d\eta_\tau}{dt} = -\lambda_\tau \eta_\tau + \mathcal{G}_\tau(t), \tag{3·18}$$

where

$$\mathcal{G}_\tau(t) \equiv \sum_{i=1}^{N} \psi_{\tau i}\, \mathcal{F}_i'(t), \tag{3·19}$$

which satisfies

$$\langle \mathcal{G}_\tau(\xi) \rangle_{\eta'} = 0, \tag{3·20}$$

$$\int_{-\infty}^{+\infty} \langle \mathcal{G}_\tau(\xi)\, \mathcal{G}_\epsilon(\xi+\tau) \rangle_{\eta'} d\tau = \sigma_{\tau\epsilon}\,. \tag{3·21}$$

The formal solution of Eq. (3·18) is given by

$$\eta_\tau(t) = \eta_\tau^* e^{-\lambda_\tau t} + \int_0^t e^{\lambda_\tau(\xi - t)}\, \mathcal{G}_\tau(\xi)\, d\xi, \tag{3·22}$$

which has the probability distribution (3·12)[8].

§ 4. Brownian motion of a colloidal particle

As the first example we shall treat the original problem of Brownian motion of a colloidal particle in an uniform isotropic medium of temperature T^0. The isolated system under consideration is composed of both the particle and the medium. For the sake of simplicity let us suppose that the variable α specifying the system be only the momentum of the particle $\boldsymbol{p} \equiv (p_x, p_y, p_z)$.

For this case the equilibrium distribution becomes the Maxwellian

$$W(\boldsymbol{p}') = (2\pi m k T^0)^{-3/2} \exp\left(-\frac{\boldsymbol{p}^2}{2mkT^0}\right), \tag{4·1}$$

where m denotes the mass of the particle. Remembering Eqs. (1·9) and (1·2), we obtain the affinity vector

$$\boldsymbol{A}(\boldsymbol{p}') = -\boldsymbol{p}'/m. \tag{4·2}$$

On the other hand, as the medium is isotropic, we may put the matrix of kinetic coefficients (L_{ij}) to be diagonal :

$$L_{ij}=f\delta_{ij} \qquad (i,j=x,y,z), \tag{4·3}$$

f being the friction constant. As the matrix (S_{ij}) is diagonal, the eigenvalue problem (3·8) is already solved, and there is no eigenvalue other than

$$\lambda=f/m. \tag{4·4}$$

Thus Fokker-Planck's equation (3·6) or (3·9) becomes

$$\frac{\partial W(\boldsymbol{p}',t)}{\partial t}=\lambda\frac{\partial}{\partial \boldsymbol{p}'}\cdot\{\boldsymbol{p}'W(\boldsymbol{p}',t)\}+D\frac{\partial^2 W(\boldsymbol{p}',t)}{\partial \boldsymbol{p}'^2}, \tag{4·5}$$

where

$$D\equiv kT^0f \tag{4·6}$$

is the diffusion coefficient in the momentum space. (The diffusion coefficient in the ordinary space is given by $D/f^2=kT^0/f$). As is well-known, the fundamental solution of (4·5) is

$$W(\boldsymbol{p}',t)=\{2\pi mkT^0(1-e^{-2\lambda t})\}^{-3/2}\exp\left[-\frac{|\boldsymbol{p}-\boldsymbol{p}^*e^{-\lambda t}|^2}{2mkT^0(1-e^{-2\lambda t})}\right]. \tag{4·7}$$

Similarly, the stochastic differential equation (3·14) or (3·18) becomes

$$\frac{d\boldsymbol{p}}{dt}=-f\frac{\boldsymbol{p}}{m}+\boldsymbol{F}(t), \tag{4·8}$$

where the fluctuating force $\boldsymbol{F}(t)$ satisfies

$$\langle \boldsymbol{F}(\xi)\rangle_{P'}=0, \tag{4·9}$$

$$\int_{-\infty}^{+\infty}\langle \boldsymbol{F}(\xi)\boldsymbol{F}(\xi+\tau)\rangle_{P'}d\tau=2D\mathbf{1}, \tag{4·10}$$

$\mathbf{1}$ being the unit tensor. These results are completely in agreement with those of the usual theory of Brownian motion.

When an external force $\boldsymbol{K}$ with a potential φ, say*

$$\boldsymbol{K}(\boldsymbol{x})=-\frac{\partial\varphi(\boldsymbol{x})}{\partial \boldsymbol{x}}, \tag{4·11}$$

acts on the particle at each position $\boldsymbol{x}$, the system becomes *non-isolated*, though is thermally isolated, for there is the mechanical work done on it. Thus our theory can not be applied to this case. However, by considering this case, we shall obtain a suggestion for the generalization of our theory to non-isolated systems.

From the Maxwell-Boltzmann distribution

$$W(\boldsymbol{x}',\boldsymbol{p}')\propto\exp\left[-\left\{\frac{\boldsymbol{p}'^2}{2m}+\varphi(\boldsymbol{x}')\right\}\Big/(kT^0)\right], \tag{4·12}$$

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* An external magnetic or Coriolis field can be treated in the similar manner. Cf. Callen[9].

we obtain the affinities*

$$(A_1, A_2, A_3) = \boldsymbol{K}(\boldsymbol{x}'), \qquad (A_4, A_5, A_6) = -\boldsymbol{p}'/m. \tag{4·13}$$

In order to get the equations of motion

$$\left.\begin{aligned} \frac{d\boldsymbol{x}'}{dt} &= \frac{\boldsymbol{p}'}{m}, \\ \frac{d\boldsymbol{p}'}{dt} &= -f\frac{\boldsymbol{p}'}{m} + \boldsymbol{K}(\boldsymbol{x}') \end{aligned}\right\} \tag{4·14}$$

from the linear equations of the type (1·3), we must assume the kinetic coefficients of the form

$$(L_{ij}) = f\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \tag{4·15}$$

which has the symmetric and the antisymmetric parts.

Thus we must in general divide the kinetic coefficient into its symmetric and antisymmetric parts :

$$\left.\begin{aligned} L_{ij} &= L_{ij}^{(s)} + L_{ij}^{(a)}, \\ L_{ij}^{(s)} &= L_{ji}^{(s)}, \quad L_{ij}^{(a)} = -L_{ji}^{(a)}. \end{aligned}\right\} \tag{4·16}$$

Then, as pointed out by Callen[9], the antisymmetric part ($L_{ij}^{(a)}$) does not contribute to the energy dissipation. On the other hand, according to the idea of Nyquist[6], the fluctuation should be coupled with the energy dissipation. From this point of view it will be natural to assume the stochastic equation of the form

$$\frac{da_i}{dt} = \sum_{j=1}^{N} L_{ij}^{(a)} A_j(a) + \sum_{j=1}^{N} L_{ij}^{(s)} \{A_j(a) + \mathcal{A}_j(a, t)\}, \tag{4·17}$$

where the statistical properties of $\mathcal{A}(a, t)$ is determined by the transition probability

$$k \log \mathcal{W}(a' \Delta t, a'') = \frac{1}{2}\left\{ (\Delta S)_{irr.} - \frac{\Phi[(\Delta a)_{irr.}, (\Delta a')_{irr.}]}{T^0 \Delta t} \right\}; \tag{4·18}$$

$$(\Delta S)_{irr.} \equiv \frac{1}{T^0} \sum_{i=1}^{N} A_i(a') (\Delta a')_{irr.} + O(\Delta t^2), \tag{4·19}$$

$$\Phi[(\Delta a')_{irr.}, (\Delta a')_{irr.}] \equiv \frac{1}{2} \sum_{i,j=1}^{N} R_{ij}^{(s)} (\Delta a_i')_{irr.} (\Delta a_j')_{irr.}, \tag{4·20}$$

$$(\Delta a_i')_{irr.} \equiv \Delta a_i' - \sum_{j=1}^{N} L_{ij}^{(a)} A_j(a') \Delta t, \tag{4·21}$$

---

* In Eq. (1·2) the entropy S has to be naturally replaced by $-F(a')/T^\circ$, F being a free energy (or, more precisely, the "minimum work" necessary to take the system out of complete equilibrium a° into the given state a').

the matrix $(R_{ij}^{(s)})$ being the reciprocal of $(L_{ij}^{(s)})$. It will be interesting to notice here that *the principle of microscopic reversibility* stated in the form

$$\langle \mathcal{A}_i(a', \xi)\mathcal{A}_j(a', \xi+\tau)\rangle_{a'} = \langle \mathcal{A}_i(a', \xi+\tau)\mathcal{A}_j(a', \xi)\rangle_{a'} \tag{4·22}$$

excludes the appearance of the antisymmetric part $(L_{ij}^{(a)})$ in Eq. (4·20) [cf. Eq. (2·20)].

§ 5. Fluctuations in heat flow

As the second example of our theory, we shall now consider the conduction of heat along an isolated rod. This problem was already treated by Ornstein and Milatz[10]. Their treatment, however, contains one essential assumption, which made their result complicated and different from ours. The problem of diffusion will be treated in the same manner[11].

For the sake of simplicity let us confine ourselves to the one-dimensional case, in which the value of temperature $T'(x)$ at a position x does not deviate so much from its equilibrium one T^0, and the approximation

$$\frac{1}{T'(x)} = \frac{1}{T^0}\left\{1 - \frac{\Delta T'(x)}{T^0}\right\}; \tag{5·1}$$

$$\Delta T'(x) \equiv T'(x) - T^0 \tag{5·2}$$

may be used. Under this approximation Casimir[12] gave the expression for the entropy

$$S[\Delta T'] = S^0 - \frac{C}{2}\int_0^L \left\{\frac{\Delta T'(x)}{T^0}\right\}^2 dx$$

$$= S^0 - \frac{1}{2}\int_0^L\int_0^L S(x, x')\Delta T'(x)\Delta T'(x')\,dx\,dx'; \tag{5·3}$$

$$S(x, x') \equiv \frac{C}{T^{0\,2}}\delta(x - x'), \tag{5·4}$$

where L denotes the length of the rod, and C the heat capacity per unit of length (assumed to be constant). If we regard $\Delta T(x)$ as the variable a_i, the theory developed in § 3 can be applied, after its generalization to the case of continuous parameters. Since the entropy (5·3) is a functional, the affinity is obtained by the functional derivative:

$$A[x\,;\,\Delta T'] \equiv T^0\frac{\delta S[\Delta T']}{\delta \Delta T'(x)} = -\frac{C}{T^0}\Delta T'(x). \tag{5·5}$$

From Eq. (1·1) we have the rate of entropy production

$$\left(\frac{dS}{dt}\right)_{irr.}[\Delta T'] = \frac{1}{T^0}\int_0^L A[x\,;\,\Delta T']\frac{\partial \Delta T'(x)}{\partial t}dx, \tag{5·6}$$

which is easily found to be equivalent to the usual expression in "the thermodynamics of irreversible processes"[1]:

$$\left(\frac{dS}{dt}\right)_{irr}[\Delta T'] = \int_0^L Q'(x)\frac{\partial}{\partial x}\left\{\frac{1}{T'(x)}\right\}dx \tag{5·7}$$

within the approximation (5·1), if we notice the equation of energy conservation and the boundary condition :

$$C\frac{\partial T'(x)}{\partial t} + \frac{\partial}{\partial x}Q'(x) = 0, \tag{5·8}$$

$$Q'(0) = Q'(L) = 0. \tag{5·9}$$

By the assumption of Fourier's law

$$Q'(x) = -\varkappa\frac{\partial T'(x)}{\partial x} \tag{5·10}$$

Eq. (5·8) becomes the well-known equation of heat conduction

$$\frac{\partial T'(x)}{\partial t} = \frac{\varkappa}{C}\frac{\partial^2 T'(x)}{\partial x^2}, \tag{5·11}$$

which can be rewritten into the integral form

$$\frac{\partial \Delta T'(x)}{\partial t} = \int_0^L L(x, x')\dot{A}[x'; \Delta T']\,dx'; \tag{5·12}$$

$$L(x, x') \equiv -\frac{\varkappa T^0}{C^2}\frac{\partial^2\delta(x-x')}{\partial x'^2} = L(x', x). \tag{5·13}$$

The equation (5·12) is just Eq. (1·3) for the present case. $\varkappa$ denotes the coefficient of heat conductivity.

As we have known the integral kernels $S(x, x')$ and $L(x, x')$, we can now develop the theory of § 3 explicitly. First we must solve the eigenvalue problem for the kernel

$$\Lambda(x, x') \equiv T^0\int_0^L L(x, x'')S(x'', x')\,dx'' = -\frac{\varkappa}{C}\frac{\partial^2\delta(x-x')}{\partial x'^2}. \tag{5·14}$$

Under the boundary condition (5·9), the eigenfunctions are

$$\sqrt{\frac{1}{L}},\ \sqrt{\frac{2}{L}}\cos\left(\frac{n\pi}{L}x\right):\ n = 1, 2, 3, \cdots, \tag{5·15}$$

from which we shall, however, *omit the first one* in order to avoid mathematical difficulties. Thus we confine ourselves to the functional space determined by the orthonormal set of eigenfunctions

$$\phi_n(x) = \sqrt{\frac{2}{L}}\cos\left(\frac{n\pi}{L}x\right),\quad n = 1, 2, 3, \cdots. \tag{5·16}$$

In this space we may put

$$\delta(x-x') = \frac{2}{L}\sum_{n=1}^{\infty}\cos\left(\frac{n\pi}{L}x\right)\cos\left(\frac{n\pi}{L}x'\right), \tag{5·17}$$

so that we have the eigenfunction expansion

$$\Lambda(x, x') = \frac{2}{L} \sum_{n=1}^{\infty} \lambda_n \cos\left(\frac{n\pi}{L} x\right) \cos\left(\frac{n\pi}{L} x'\right), \tag{5·18}$$

where the eigenvalues are

$$\lambda_n = \frac{\varkappa}{C}\left(\frac{n\pi}{L}\right)^2, \quad n = 1, 2, 3, \cdots. \tag{5·19}$$

The transformation (3·7) becomes

$$\left.\begin{aligned} \eta_n &= \sqrt{\frac{2}{L}} \int_0^L \Delta T(x) \cos\left(\frac{n\pi}{L} x\right) dx, \\ \Delta T(x) &= \sqrt{\frac{2}{L}} \sum_{n=1}^{\infty} \eta_n \cos\left(\frac{n\pi}{L} x\right). \end{aligned}\right\} \tag{5·20}$$

Similarly the matrix element (3·10) becomes

$$\begin{aligned} \sigma_{n,m} &\equiv 2 \int_0^L \int_0^L k T^0 L(x, x') \psi_n(x) \psi_m(x') dx dx' \\ &= 2 \frac{k T^{02}}{C} \lambda_n \delta_{n,m}. \end{aligned} \tag{5·21}$$

In Ornstein-Milatz theory[10] this $\sigma_{n,m}$ was *assumed* to be of the form $\sigma \delta_{n,m}$, where the diagonal element σ is a constant *independent of* n. Such an assumption will contradict Onsager's principle. Since our matrix $(\sigma_{n,m})$ is diagonal, we can compute the reciprocal of the matrix defined by Eq. (3·13):

$$\Gamma_{n,m} = \frac{C}{k T^{02}} \frac{\delta_{n,m}}{1 - \exp(-2\lambda_n t)}, \tag{5·22}$$

which gives in turn the probability distribution of η:

$$W(\eta', t) = \prod_{n=1}^{\infty} \left[2\pi \frac{k T^{02}}{C}\left(1 - e^{-2\lambda_n t}\right)\right]^{-1/2} \exp\left[-\frac{(\eta_n - \eta_n^* e^{-\lambda_n t})^2}{2 \frac{k T^{02}}{C}\left(1 - e^{-2\lambda_n t}\right)}\right]. \tag{5·23}$$

If we may make use of the kernel (5·14), we can express the preceding distribution in terms of the original variables $\Delta T'(x)$. For this purpose we utilize the eigenfunction expansion

$$(f[\Lambda])(x, x') = \frac{2}{L} \sum_{n=1}^{\infty} f(\lambda_n) \cos\left(\frac{n\pi}{L} x\right) \cos\left(\frac{n\pi}{L} x'\right) \tag{5·24}$$

for any function $f(\lambda)$ that can be expanded in a power series of λ. For example, representing the average with respect to $W[\Delta T'; t]$ or $W(\eta', t)$ by $\langle \cdots \rangle_t$, we have

$$\langle \Delta T(x) \rangle_t = \sqrt{\frac{2}{L}} \sum_{n=1}^{\infty} \langle \eta_n \rangle_t \cos\left(\frac{n\pi}{L} x\right)$$

$$=\sqrt{\frac{2}{L}}\sum_{n=1}^{\infty}\eta_n^* e^{-\lambda_n t}\cos\left(\frac{n\pi}{L}x\right)$$

$$=\int_0^L \Delta T^*(x')\,(e^{-\Delta t})\,(x', x)\,dx', \tag{5·25}$$

where $\Delta T^*(x)$ denotes the given initial temperature distribution

$$\Delta T^*(x)=\sqrt{\frac{2}{L}}\sum_{n=1}^{\infty}\eta_n^*\cos\left(\frac{n\pi}{L}x\right). \tag{5·26}$$

In the same way, we obtain the variances

$$\langle\{\Delta T(x)-\langle\Delta T(x)\rangle_t\}\{\Delta T(x')-\langle\Delta T(x')\rangle_t\}\rangle_t$$

$$=\frac{2}{L}\sum_{n,m=1}^{\infty}\langle(\eta_n-\langle\eta_n\rangle_t)(\eta_m-\langle\eta_m\rangle_t)\rangle_t\cos\left(\frac{n\pi}{L}x\right)\cos\left(\frac{m\pi}{L}x'\right)$$

$$=\frac{kT^{02}}{C}\frac{2}{L}\sum_{n=1}^{\infty}(1-e^{-2\lambda_n t})\cos\left(\frac{n\pi}{L}x\right)\cos\left(\frac{n\pi}{L}x'\right)$$

$$=\frac{kT^{02}}{C}(1-e^{-2\Delta t})\,(x, x'). \tag{5·27}$$

As is readily seen, in the limit $t\to\infty$ these averages and variances approach the usual results[12]:

$$\left.\begin{aligned}&\langle\Delta T(x)\rangle_\infty=0,\\&\langle\Delta T(x)\,\Delta T(x')\rangle_\infty=\frac{kT^{02}}{C}\delta(x-x').\end{aligned}\right\} \tag{5·28}$$

Making use of the expressions (5·25) and (5·27), we can at once write down the probability distribution for $\Delta T(x)$

$$W[\Delta T';\,t]=N(t)\exp\left[-\frac{C}{2kT^{02}}\int_0^L\int_0^L\left(\frac{1}{1-e^{-2\Delta t}}\right)(x, x')\right.$$

$$\left.\cdot\{\Delta T'(x)-\langle\Delta T(x)\rangle_t\}\{\Delta T'(x')-\langle\Delta T(x')\rangle_t\}\,dx\,dx'\right], \tag{5·29}$$

where $N(t)$ is the normalization factor

$$N(t)=\prod_{n=1}^{\infty}\left[2\pi\frac{kT^{02}}{C}(1-e^{-2\lambda_n t})\right]^{-1/2}, \tag{5·30}$$

which, unfortunately, becomes infinite. In order to obtain the finite $N(t)$ we should have cut off the higher Fourier components of $\Delta T'(x)$. The expression (5·29) reduces to the equilibrium distribution (1·9) with the entropy (5·3) in the limit $t\to\infty$, as it should be.

To compute the correlation between the variables at different times or the spectrum of $\Delta T(x)$, in addition to our general theory, we must know in general the details of

the fluctuation spectrum of $\mathcal{A}(t)$. In fact, from Eqs. (5·20) and (3·22), we have

$$\Delta T(x,t)=\sqrt{\frac{2}{L}}\sum_{n=1}^{\infty}\left\{\eta_n^* e^{-\lambda_n t}+\int_0^t e^{\lambda_n(\xi-t)}\mathcal{G}_n(\xi)d\xi\right\}\cos\left(\frac{n\pi}{L}x\right); \tag{5·31}$$

$$\langle \mathcal{G}_n(\xi)\rangle_{\eta'}=0, \tag{5·32}$$

$$\int_{-\infty}^{+\infty}\langle \mathcal{G}_n(\xi)\mathcal{G}_m(\xi+\tau)\rangle_{\eta'}d\tau=\sigma_{n,m}, \tag{5·33}$$

and hence

$$\langle \Delta T(x,s)\rangle_{\Delta T'}=\sqrt{\frac{2}{L}}\sum_{n=1}^{\infty}\eta_n^* e^{-\lambda_n}\cos\left(\frac{n\pi}{L}x\right)=\langle \Delta T(x)\rangle_t, \tag{5·34}$$

where the average $\langle\cdots\rangle_{\Delta T'}$ has the same meaning as that of $\langle\cdots\rangle_{\alpha'}$ in Eq. (2·17). Similarly, for a sufficiently large $\tau(>0)$ compared with Δt we have

$$\begin{aligned}
&\langle\{\Delta T(x,s)-\langle\Delta T(x)\rangle_t\}\{\Delta T(x',s+\tau)-\langle\Delta T(x')\rangle_{t+\tau}\}\rangle_{\Delta T'}\\
&=\frac{2}{L}\sum_{n,m=1}^{\infty}\cos\left(\frac{n\pi}{L}x\right)\cos\left(\frac{m\pi}{L}x'\right)\int_0^t d\xi\int_0^{t+\tau}d\xi' e^{\lambda_n(\xi-t)}e^{\lambda_m(\xi'-t-\tau)}\langle\mathcal{G}_n(\xi)\mathcal{G}_m(\xi')\rangle_{\eta'}\\
&=\frac{2}{L}\sum_{n,m=1}^{\infty}e^{-\lambda_m\tau}\cos\left(\frac{n\pi}{L}x\right)\cos\left(\frac{m\pi}{L}x'\right)\int_{-t}^{0}e^{(\lambda_n+\lambda_m)u}du\\
&\qquad\cdot\int_{-\infty}^{+\infty}e^{-(\lambda_n-\lambda_m)v/2}\langle\mathcal{G}_n(\xi)\mathcal{G}_m(\xi+v)\rangle_{\eta'}dv
\end{aligned} \tag{5·35}$$

approximately. It will be seen that our result (5·33) is not sufficient for the last integration in Eq. (5·35). However, if the integrand itself of Eq. (5·33) may be assumed to contain the factor $\delta_{n,m}$ of Eq. (5·21), we can carry out the integration:

$$\begin{aligned}
&\langle\{\Delta T(x,s)-\langle\Delta T(x)\rangle_t\}\{\Delta T(x',s+\tau)-\langle\Delta T(x')\rangle_{t+\tau}\}\rangle_{\Delta T'}\\
&\quad=\frac{kT^{02}}{C}\frac{2}{L}\sum_{n=1}^{\infty}e^{-\lambda_n\tau}(1-e^{-2\lambda_n t})\cos\left(\frac{n\pi}{L}x\right)\cos\left(\frac{n\pi}{L}x'\right)\\
&\quad=\frac{kT^{02}}{C}\rho_t(x,\tau,x'),
\end{aligned} \tag{5·36}$$

where we have defined

$$\rho_t(x,\tau,x')=(e^{-\Delta\tau}[1-e^{-2\Delta t}])(x,x'). \tag{5·37}$$

The expression (5·36) reduces to Eq. (5·27) in the limit $\tau\to\infty$. It will be interesting to note here that $\rho_t(x,\tau,x')$ satisfies the original equation of heat conduction:

$$\frac{\partial\rho_t(x,\tau,x')}{\partial\tau}=\frac{\varkappa}{C}\frac{\partial^2\rho_t(x,\tau,x')}{\partial x'^2}. \tag{5·38}$$

This suggests the existence of some relations between the fluctuations in heat flow and those in phonon diffusion[12]. From Eq. (5·36) we obtain the spectral density matrix (not normalized) for $\Delta T(x)$[14)11)]:

$$G_\omega(x, x') \equiv \int_0^\infty \langle \{\Delta T(x, s) - \langle \Delta T(x) \rangle_t\}$$

$$\cdot \{\Delta T(x', s+\tau) - \langle \Delta T(x') \rangle_{t+\tau}\} \rangle_{\Delta T^0} \cos(\omega\tau) d\tau$$

$$= \frac{kT^{02}}{C} \frac{2}{L} \sum_{n=1}^{\infty} \frac{\lambda_n}{\omega^2 + \lambda_n^2} (1 - e^{-2\lambda_n t}) \cos\left(\frac{n\pi}{L} x\right) \cos\left(\frac{n\pi}{L} x'\right)$$

$$= \frac{kT^{02}}{C} \left(\frac{\Lambda}{\omega^2 + \Lambda^2} [1 - e^{-2\Lambda t}] \right)(x, x'), \tag{5·39}$$

the normalization factor of which is the reciprocal of

$$\int_0^\infty G_\omega(x, x') d\omega = \frac{kT^{02}}{C} \frac{\pi}{2} (1 - e^{-2\Lambda t})(x, x'). \tag{5·40}$$

Thus we shall see that, under our previous assumption employed in the derivation of Eq. (5·36), the normalized spectral density matrix does not depend on the equilibrium temperature T^0, and is determined only by the quantity $\varkappa/(CL^2)$.

§ 6. Concluding remarks

We have shown that, for isolated linear dissipative systems, a general statistical theory can be constructed semi-empirically to a certain extent on the basis of Onsager's principle (1·10).

The essential approximation in our theory lies, however, in the use of the definition of entropy given by the ordinary thermodynamics of non-uniform systems. In fact we have always made use of the same functional form of entropy $S(\alpha')$ whether the probability distribution of α is the equilibrium one, $W(\alpha')$, or the non-equilibrium one, $W(\alpha', t)$. This is expressed most explicitly in our use of affinity $A(\alpha')$ defined by Eq. (1·2), i.e., in Eq. (1·1) or (2·8). As was stated in § 2, this procedure is, however, closely related to the method of Boltzmann in statistical mechanics, and can be applied only when each small part of the system under consideration contains a very large number of particles. Thus our whole theory can be applied only to such systems, but is hoped to be useful to analyse semi-empirically fluctuation phenomena in irreversible processes, especially those in the neighbourhood of transition points.

References

1) For example, I. Prigogine, *Etude thermodynamique des processus irréversibles*, Liège, 1947; M. Sugita, *Thermodynamics of Transient Phenomena* (in Japanese), Tokyo, 1950; S. R. de Groot, *Thermodynamics of Irreversible Processes*, Amsterdam, 1951.
2) For example, R. Fürth, *Schwankungsershe'nungen in der Physik*, Sammlung Vieweg. Hft. 48, 1920.
3) L. Onsager, Phys. Rev. **37** (1931), 405; **38** (1931), 2265.
4) H. B. G. Casimir, Rev. Mod. Phys. **17** (1945), 343, Eq. (15).
5) For example, S. Candrasekhar, Rev. Mod. Phys. **15** (1943), 1, Eqs. (218) and (224).
6) J. B. Johnson, Phys. Rev. **32** (1928), 97; H. Nyquist, *ibid.* p. 110.
7) M. C. Wang and G. E. Uhlenbeck, Rev. Mod. Phys. **17** (1945), 323, § 11.
8) Cf., S. Chandrasekhar, *loc. cit.*, Cap. II.
9) H. B. Callen, Thesis, M. I. T., Cambridge Mass., 1947, § 10–c.
10) L. S. Ornstein and J. M. W. Milatz, Physica **6** (1939), 1139.
11) Cf., J. M. Richardson, Bell Sys. Tech. Jour. **29** (1950), 117.
12) H. B. G. Casimir, *loc. cit.*, § 4.
13) J. M. Richardson, *loc. cit.*, § 4.
14) M. C. Wang and G. E. Uhlenbeck, *loc. cit.*, § 4.

Note added in proof: After submitting my manuscript I could read the very interesting work of M. S. Green [J. Chem. Phys. **20** (1952) 1281]. He has started from the Kirkwood theory and fairly clarified irreversible phenomena from the microscopic view, while my theory based on the Onsager's is a semi-empirical one and is discussed from the macroscopic view. Though the relations in the former theory are more general than those in the latter, both theories have many points in common. Especially, Green's equation

$$\int_0^\infty [\langle v_i v_j(\sigma)\rangle - \langle v_i\rangle\langle v_j\rangle]\, d\sigma = \xi_{ij} \qquad (\sigma \gg \theta)$$

seems to coincide with my somewhat obscure relation (2·20), or more directly, (3·17). And when $\langle v_i\rangle = 0$ and $\xi_{ij} = \text{const.}$, his equation (30)

$$\frac{\partial T}{\partial t} = \sum_i \frac{\partial}{\partial a_i}\left[-\left(\langle v_i\rangle + \sum_j \frac{1}{W}\frac{\partial}{\partial a_j}[W\xi_{ji}]\right)T + \sum_j \frac{\partial}{\partial a_j}(\bar{\xi}_{ij}T)\right],$$

$$\bar{\xi}_{ij} \equiv \frac{1}{2}[\xi_{ij} + \xi_{ji}] = \bar{\xi}_{ji},$$

agrees with the Fokker-Planck equation in my theory

$$\frac{\partial W}{\partial t} + \sum_{i,j=1}^{n} \frac{\partial}{\partial a_{i'}}[L^{(a)}{}_{ij} A_j W] = \sum_{i,j=1}^{n} \frac{\partial}{\partial a_{i'}}\left[D_{ij}\left(\frac{\partial W}{\partial a_{j'}} - \frac{A_j W}{kT^0}\right)\right],$$

$$D_{ij} \equiv kT^0 L^{(s)}{}_{ij} = kT^0 (R^{(s)-1})_{ij},$$

which is derived by making use of my expression (4·18). This will support the way of the omission of the antisymmetric part $L^{(a)}$ in my theory. The definition of entropy proposed by Green seems, however, to be different from the usual one in the thermodynamics of non-uniform systems, in which man utilizes the additive property of entropy.

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The Effect of Damping on Radiative Corrections to Electron Scattering and the Problem of Infra-red Catastrophe

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The reaction of radiation on the scattering of electrons with radiative corrections is treated on the basis of covariant theory of radiation damping. It is shown that the ultra-violet divergences are removed by the process of usual mass and charge renormalisations; and the infra-red divergence, which still persists in the second order corrections to radiationless electron scattering is exactly compensated by the corresponding divergence occurring in the scattering with the emission of radiation. In § 1 the interaction Hamiltonian for the scattering processes are given after Feynman-Dyson formalism. In § 2 the covariant formulation of radiation damping and the scattering cross-sections are given. The § 3 deals with the infra-red divergences involved in the electron scattering.

Introduction

The problem of infra-red catastrophe in electron scattering and its interpretation by Bloch and Nordsieck,[1] Pauli and Fierz,[2] and Braunbek and Weinmann[3] showed for the first time the significant part played by the virtual quanta accompanying the electrons and the inadequacy of the customary perturbation theory where use is made of expansion in powers of $\alpha=e^2/4\pi\hbar c$. By making use of a canonical transformation these authors were able to include the virtual quanta in defining the state of the electron in closed form, at least in non-relativistic approximation, without expansion of the series in powers of α. It was thereby shown that the infra-red divergence associated with the scattering of electron with the emission of radiation was exactly compensated by the radiative corrections to electron scattering without radiation. It was further clarified by Pauli and Fierz that the compensation takes place only for the emission of quanta of low frequencies. But for the emission of high frequency virtual quanta involving energies higher than the electron's kinetic energy we are faced with new divergences (ultra-violet) which are again logarithmic and remain uncompensated, there being no corresponding ultra-violet term in the radiative scattering probability. The origin of new divergent terms was investigated by Dancoff[4] and Lewis[5] from relativistic considerations. It was shown by Lewis that they are all attributed to divergent mass increase of the electron. The work of Bethe and Oppenheimer[6] further revealed a new difficulty as regards the compensation of the infra-red divergent terms. They showed that the complete compensation does not take place when one takes account of the effect of the radiation damping on the electron scattering by the perturbation method of Heitler[7] and Wilson.[8] It has been, however, recently shown by

one of us[9] that the application of the theory of radiation damping as proposed by Heitler and formulated by Pauli,[10] when properly modified to take account of radiative corrections, removes completely the infra-red divergence difficulties pointed out by Bethe and Oppenheimer, at least up to the order of α. Recently a new formulation of a covariant electrodynamics has been developed by Tomonaga[11] and Schwinger[12] which gives a powerful and consistent method for investigating the radiative corrections successfully up to any order of approximations, and in which the ultra-violet divergences causing serious difficulties in previous calculations are removed unambiguously by the process of charge and mass renormalisations. It has been already shown by Schwinger that in the new quantum electrodynamics the infra-red divergence, which is left out after mass and charge renormalisations in the second order corrections to radiationless electron scattering, compensates the infra-red divergence involved in the scattering with the emission of radiation. Schwinger has, however, not considered the effect of the radiation damping on the electron scattering. In present paper we shall extend Schwinger's calculations to study the effect or radiation damping on the problem of electron scattering by a time independent scalar field and show that the scattering in this case also becomes completely free from divergences, infra-red or ultra-violet, after the usual charge and mass renormalisations. Contrary to Bethe and Oppenheimer, the infra-red divergences involved in the scattering with radiation is still being cancelled by the corresponding term due to the scattering without the emission of radiation, the extra term needed for the compensation being supplied by the higher order radiative corrections. In the first article we shall briefly work out the interaction Hamiltonian for the scattering processes after Feynman-Dyson formalism. In the second article the theory of radiation damping and scattering cross-section will be given. In the third article we shall discuss the problem of the infra-red divergences involved in the radiative corrections to electron scattering when radiation damping is taken into account.

§ 1. Covariant formulation of interaction Hamiltonian

We shall first derive briefly Schwinger results for the interaction of an electron with the electromagnetic field from the Feynman-Dyson formalism. Fig. 1, gives the lowest order elastic scattering of an electron by an external field and the corresponding matrix element is

$$H(x_0) = -ie\bar{\psi}(x_0)\gamma_\mu\psi(x_0)A^e_\mu(x_0). \qquad (1)$$

Fig. 1

The diagrams describing the second order radiative corrections to the electron scattering are obtained by introducing the vacuum polarisation, self-energy and the vertex parts to the Fig. 1 as shown in Fig. 2.

The matrix elements of various processes of Fig. 2 are given by

$$H^{(a)}_{\text{vac}}(x_0) = \frac{ie\alpha\pi}{2}\int dx_1 dx_2 \,\text{Spur}\left(\gamma_\mu S_F(x_0-x_1)\gamma_\nu S_F(x_1-x_0)\right)$$
$$\times A^e_\mu(x_0)D_F(x_1-x_2)\bar{\psi}(x_2)\gamma_\nu\psi(x_2), \qquad (2)$$

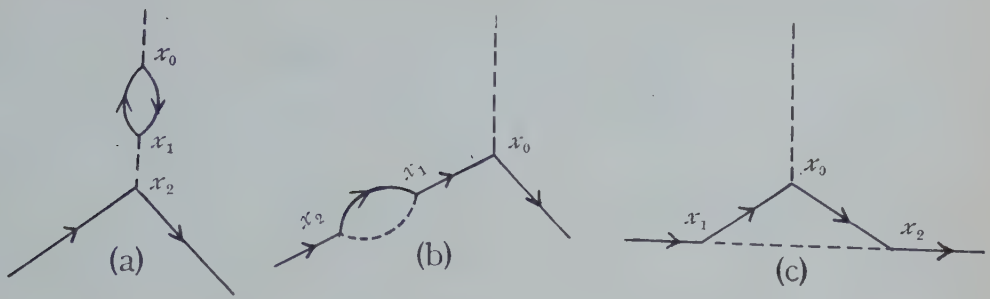

Fig. 2

$$H^{(b)}_{\text{self}}(x_0) = -\frac{ie\alpha\pi}{2}\int dx_1 dx_2\, A^e_\mu(x_0)[\bar\psi(x_0)\gamma_\mu S_F(x_1-x_0)\gamma_\nu S_F(x_2-x_1)\gamma_\nu\psi(x_2)$$
$$\times D_F(x_2-x_1) + \bar\psi(x_2)\gamma_\nu S_F(x_1-x_2)\gamma_\nu D_F(x_1-x_2)\, S_F(x_0-x_1)\gamma_\mu\psi(x_0)]$$
$$-\frac{e}{2\hbar}\delta mc\int dx_1 A^e_\mu(x_0)[\bar\psi(x_0)\gamma_\mu S_F(x_1-x_0)\psi(x_1)$$
$$+\psi(x_1)\, S_F(x_0-x_1)\gamma_\mu\psi(x_0)], \qquad (3)$$

$$H^{(c)}_{\text{vertex}}(x_0) = -\frac{ie\alpha\pi}{2}\int dx_1 dx_2 A^e_\mu(x_0)[\bar\psi(x_1)\gamma_\nu S_F(x_0-x_1)\gamma_\mu S_F(x_2-x_0)$$
$$\times\gamma_\nu\psi(x_2)]\, D_F(x_1-x_2), \qquad (4)$$

where $\alpha=e^2/4\pi\hbar c$ and $D_F(x)$ and $S_F(x)$ are Feynman's functions for the electromagnetic field and electron respectively and given by

$$D_F(x) = \frac{-2i}{(2\pi)^4}\int\frac{e^{-ipx}}{p^2+\lambda^2}dp\,; \quad S_F(x) = \frac{-2i}{(2\pi)^4}\int e^{-ipx}dp\,\frac{i\gamma p-\varkappa_0}{p^2+\varkappa_0^2}. \qquad (5)$$

λ is introduced in $D_F(x)$ to avoid the anticipated infra-red divergences and will be made to $\to 0$ after all operations are performed. Similarly the lowest order matrix element for bremsstrahlung is obtained from the Fig. 3 and is given by

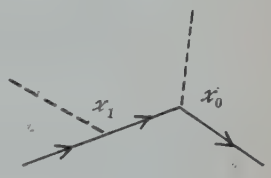

Fig. 3

$$H^{(1)}(x_0) = \frac{ie^2}{2\hbar c}\int dx_1[\bar\psi(x_0)\gamma_\mu S_F(x_1-x_0)\gamma_\nu\psi(x_1)$$
$$+\bar\psi(x_1)\gamma_\nu S_F(x_0-x_1)\gamma_\mu\psi(x_0)]A^e_\mu(x_0)A_\nu(x_1), \qquad (6)$$

where $A^e_\mu(x_0)$ is the external field and $A_\nu(x_1)$ the electromagnetic field.

We now proceed to calculate the second order corrections to the charge-current. The charge-current due to the vacuum polarisation can be expressed as

$$\delta j^a_\mu(x_0) = i\pi\alpha c\int dx_1 G_{\mu\nu}(x_0-x_1)\,\delta A_\nu(x_1), \qquad (7)$$

where

$$\delta A_\nu(x_1) = -e/2\int dx_2 D_F(x_1-x_2)\bar\psi(x_2)\gamma_\nu\psi(x_2), \qquad (8)$$

and

$$G_{\mu\nu}(x) = \text{Spur}\{\gamma_\mu S_F(x)\gamma_\nu S_F(-x)\}. \tag{9}$$

Now by making the Fourier integral representation of $S_F(x)$ and evaluating the spurs we can write

$$G_{\mu\nu}(x) = \frac{-16}{(2\pi)^8}\int dk'\,dk''\,e^{ix(k'+k'')}\,\frac{k_\mu' k_\nu'' + k_\mu'' k_\nu' - \delta_{\mu\nu}(k'k'' - \varkappa_0^2)}{(k'^2+\varkappa_0^2)(k''^2+\varkappa_0^2)}. \tag{10}$$

It is easily seen that the requirements of charge conservation and gauge invariance are satisfied if

$$\int \frac{k_\nu' dk'}{k'^2+\varkappa_0^2} = 0\,, \quad \int \frac{k_\nu'' dk''}{k''^2+\varkappa_0^2} = 0. \tag{11}$$

Introducing new variables k_μ and p_μ defined by

$$k_\mu' = \frac{1}{2}k_\mu(1-v) + p_\mu\,, \quad k_\mu'' = \frac{1}{2}k_\mu(1+v) - p_\mu\,, \tag{12}$$

and writing

$$\frac{1}{(k''^2+\varkappa_0^2)(k'^2+\varkappa_0^2)} = \frac{1}{2}\int_{-1}^{+1} dv\left[\frac{k'^2+k''^2}{2} + \frac{v}{2}(k'^2-k''^2) + \varkappa_0^2\right]^{-2}, \tag{13}$$

we obtain, following Schwinger

$$G_{\mu\nu}(x) = \left(\frac{\partial^2}{\partial x_\mu \partial x_\nu} - \delta_{\mu\nu}\Box^2\right)G_1(x), \tag{14}$$

where

$$G_1(x) = \frac{4}{(2\pi)^8}\int_{-1}^{+1} dv(1-v^2)\int dk\,dp\,e^{ikx}\left(\varkappa_0^2 + p^2 + \frac{k^2}{4}(1-v^2)\right)^{-2} \tag{15}$$

$$= \frac{2i}{3\pi^2}\,Lt_{P\to\infty}\left(\log\frac{P+P_0}{\varkappa_0} - 1\right)\delta(x) + \frac{2i}{8\pi^2\varkappa_0^2}\Box^2\left(F_1(x) - \frac{1}{3}F_2(x)\right) \tag{16}$$

by a partial integration with respect to v.

The expression (7) for the charge-current is thus reduced to

$$\delta j_\mu^a(x_0) = \frac{-2a}{3\pi}\left(Lt_{P\to\infty}\log\frac{P+P_0}{\varkappa_0} - 1\right)J_\mu(x_0) - \frac{2a}{8\pi\varkappa_0^2}\int \Box^2\Big(F_1(x_0-x_1) - \frac{1}{3}F_2(x_0-x_1)\Big)J_\mu(x_1)\,dx_1\,, \tag{17}$$

where

$$F_n(x) = \int_0^1 v^{2n}\,dv\,\frac{1}{(2\pi)^4}\int \frac{e^{ikx}\,dk}{1+(k^2/4\varkappa_0^2)(1-v^2)}\,, \tag{18}$$

and

$$P_0 = \sqrt{P^2+\varkappa_0^2}. \tag{19}$$

The diagram (b) corresponding the self-energy part gives rise only to mass and

charge renormalisations. The charge-current corresponding to this diagram is given by

$$\delta j_\mu^b(x_0) = \frac{i\pi ue c}{2}\int dx_1 dx_2 [\bar\psi(x_0)\gamma_\mu S_F(x_1-x_0)K(x_2-x_1)\psi(x_2)$$
$$+\bar\psi(x_2)K(x_1-x_2)S_F(x_0-x_1)\gamma_\mu\psi(x_0)]$$
$$+\frac{e}{2\hbar}\,\delta mc^2\int dx_1[\bar\psi(x_0)\gamma_\mu S_F(x_1-x_0)\psi(x_1)+\psi(x_1)S_F(x_0-x_1)\gamma_\mu\psi(x_0)], \quad (20)$$

where $K(x)$ is given by:—

$$K(x) = \frac{-4}{(2\pi)^8}\int dk\,dp\,\frac{e^{-ipx}\gamma_\nu\{i\gamma(p-k)-\varkappa_0\}\gamma_\nu}{[(p-k)^2+\varkappa_0^2](k^2+\lambda^2)}. \quad (21)$$

Now since

$$\frac{1}{[(p-k)^2+\varkappa_0^2][k^2+\lambda^2]} = \int_0^1 du[(k-up)^2+\varkappa_0^2u^2+\lambda^2(1-u)+u(1-u)(p^2+\varkappa_0^2)]^{-2}, \quad (22)$$

the transformation

$$k_\mu \to k_\mu + up_\mu \quad (23)$$

brings $K(x)$ into the form

$$K(x) = \frac{8}{(2\pi)^8}\int dk\,dp\,e^{-ipx}\int_0^1 du\left(1-up_\mu\frac{\partial}{\partial k_\mu}\right)$$
$$\times\left[\frac{i\gamma p(1-u)-i\gamma k+2\varkappa_0}{\{k^2+u^2\varkappa_0^2+\lambda^2(1-u)+(p^2+\varkappa_0^2)u(1-u)\}^2}\right]. \quad (24)$$

Here the first derivative in the integrand represents the contributions from a surface term which must be added to take into account the effect of the displacement (23) at large values of $|k|$ where the integrand does not tend to zero rapidly enough. Taking

$$\int k_\mu f(k^2)\,dk = 0\,, \quad \int k_\mu k_\nu f(k^2)\,dk = \frac{1}{4}\,\delta_{\mu\nu}\int k^2 f(k^2)\,dk\,,$$

and simplifying and rearranging terms as done by Karplus and Kroll[12] we obtain finally

$$K(x) = \frac{8}{(2\pi)^8}\int dp\,e^{-ipx}\int_0^1 du\left[\left\{\int\frac{(1+u)\varkappa_0\,dk}{(k^2+\Lambda_0^2)^2}-\frac{i\pi^2\varkappa_0}{4}\right\}\right.$$
$$\left.+(i\gamma p+\varkappa_0)(1-u)\left\{\int\frac{dk}{(k^2+\Lambda_0^2)^2}-\frac{2i\pi^2\varkappa_0^2u(1+u)}{\Lambda_0^2}+\frac{i\pi^2}{2}\right\}\right]. \quad (25)$$

Now substituting (25) in (20) and evaluating the integrals in the usual way, the first term which contributes to the self-energy cancels with the counter self-energy term as given by the last term of (20). We thus obtain finally, after replacing the renormalisation factor Z_2 by $Z_2^{1/2}$, as shown by Karplus and Kroll,

$$\delta j_\mu^b(x_0) = \frac{\alpha}{2\pi}\left(2\log\frac{\varkappa_0}{2k_{\min}}-\log\frac{P+P_0}{\varkappa_0}+\frac{3}{4}\right)J_\mu(x_0), \quad (26)$$

where we have used the relation

$$e\lambda = 2k_{\min} . \tag{26a}$$

This is proportional to the current operator and therefore can be removed by the procedure of charge renormalisation. It will, however, be shown that this cancels with the term from the vertex part when we add them together to obtain the total current.

We now calculate the contribution to the current arising from vertex part :

$$\delta j_\mu^c(x_0) = \frac{i\pi ae c}{2} \int dx_1 dx_2 \bar{\psi}(x_1) K_\mu(x_0 - x_1, x_2 - x_0) \psi(x_2) \tag{27}$$

where

$$K_\mu(x_0 - x_1, x_2 - x_0) = D_F(x_1 - x_2)\gamma_\nu S_F(x_0 - x_1)\gamma_\mu S_F(x_2 - x_0)\gamma_\nu . \tag{28}$$

By making the Fourier integral representation and proceeding in the usual way we can express (28) as

$$K_\mu(x_0 - x_1, x_2 - x_0) = \left[\frac{-2i}{(2\pi)^4}\right]^3 \int dx_1 dx_2 dk\, dk'\, dk''\, e^{-ik(x_1 - x_2)}\, e^{-ik'(x_0 - x_1)}$$

$$\times e^{-ik''(x_2 - x_0)} \times \frac{\bar{\psi}(x_1)\gamma_\nu(i\gamma k' - \varkappa_0)\gamma_\mu(i\gamma k'' - \varkappa_0)\gamma_\nu \psi(x_2)}{(k^2 + \lambda^2)(k'^2 + \varkappa_0^2)(k''^2 + \varkappa_0^2)} . \tag{29}$$

We now introduce the variables

$$p_\mu' = k_\mu' - k_\mu , \quad p_\mu'' = k_\mu'' - k_\mu , \tag{30}$$

and note that $\bar{\psi}(x_1)$ and $\psi(x_2)$ occur on the left and right respectively and that the integrations are performed with respect to x_1 and x_2. This means that only values of p_μ' and p_μ'' should occur for which $p'^2 + \varkappa_0^2 = p''^2 + \varkappa_0^2 = 0$, and $(i\gamma p' + \varkappa_0)$ (on left) $= 0$ and $(i\gamma p'' + \varkappa_0)$ (on right) $= 0$.

As a result of this transformation (29) becomes

$$K_\mu(x_0 - x_1, x_2 - x_0) = \left[\frac{-2i}{(2\pi)^4}\right]^3 \int dk\, dp'\, dp'' \cdot e^{ip'(x_1 - x_0)}\, e^{ip''(x_0 - x_2)}$$

$$\times \frac{\gamma_\nu(i\gamma(p' + \varkappa) - \varkappa_0)\gamma_\mu(i\gamma(p'' + k) - \varkappa_0)\gamma_\nu}{(k^2 + 2kp')(k^2 + 2kp'')(k^2 + \lambda^2)} . \tag{31}$$

Writing now

$$\frac{1}{(k^2 + 2p'k)(k^2 + 2p''k)(k^2 + \lambda^2)} = \int_0^1 u\,du \int_{-1}^{+1} dv \left[k^2 + \lambda^2(1-u) + ku\{(p' + p'') + v(p'' - p')\}\right]^{-3} \tag{32}$$

and making the transformation

$$k_\mu \to k_\mu - \frac{u}{2}\{(p_\mu' + p_\mu'') + v(p_\mu'' - p_\mu')\}, \tag{33}$$

we obtain

$$K_\mu(x_0-x_1, x_2-x_0)=\left[\frac{-2i}{(2\pi)^4}\right]^3\int dk\,dp'\,dp''\cdot e^{ip'(x_1-x_0)}\,e^{ip''(x_0-x_2)}\int_0^1 du u\int_{-1}^{+1}dv$$
$$\times\frac{\gamma_\nu[i\gamma\{k+p'-u/2(p'+p''+v(p''-p'))\}-x_0]}{(k^2+\Lambda^2)^3}$$
$$\times\gamma_\mu[i\gamma\{k+p''-u/2(p'+p''+v(p''-p'))\}-x_0]\gamma_\nu \tag{34}$$

where

$$\Lambda^2=\Lambda_0^2+\frac{u^2(1-v^2)}{4}(p'-p'')^2,\quad \Lambda_0^2=u^2x_0^2+\lambda(1-u). \tag{35}$$

Here no surface term is necessary since the divergence is only logarithmic.

In evaluating the integral we note the symmetry of the denominator with respect to k–integration and discard terms linear in k_λ which do not contribute, while replace $k_\lambda k_\sigma$ by $(1/4)\delta_{\lambda\sigma}k^2$. After these simplifications the factor involving γ's in (34) becomes

$$\gamma_\nu\left[i\gamma\left(p'-\frac{u(p'+p'')}{2}-\frac{uv}{2}(p''-p')\right)-x_0\right]$$
$$\times\gamma_\mu\left[i\gamma\left(p''-\frac{u}{2}(p'+p'')-\frac{uv}{2}(p''-p')\right)-x_0\right]\gamma_\nu-k^2\gamma_\mu. \tag{36}$$

This expression has already been obtained by Schwinger[12] and following him we can write after performing the integrations

$$K_\mu(x_0-x_1, x_2-x_0)=-\frac{1}{\pi^2}\delta(x_0-x_2)\gamma_\mu\left[2\log\frac{x_0}{\lambda}-\frac{5}{4}-\underset{P\to\infty}{Lt}\log\frac{P+P_0}{x_0}\right]\delta(x_1-x_0)$$
$$+\frac{2}{4\pi^2}\gamma_\mu\delta(x_1-x_2)\frac{\Box^2}{x_0^2}\left[\log\frac{x_0}{2k_{\min}}(F_0(x_0-x_1)+F_1(x_0-x_1))+\frac{1}{2}F_0(x_0-x_1)\right.$$
$$\left.+F_1(x_0-x_1)+\frac{1}{2}G(x_0-x_1)\right]-\frac{2i}{4\pi^2}\delta(x_1-x_2)\sigma_{\mu\nu}\frac{\partial}{\partial x_{0\nu}}F_0(x_0-x_1). \tag{37}$$

Substituting (37) in (27) we obtain finally

$$\delta j_\mu^c(x_0)=-\frac{a}{2\pi}\left[2\log\frac{x_0}{2k_{\min}}+\frac{3}{4}-\log\frac{P+P_0}{x_0}\right]J_\mu(x_0)$$
$$+\frac{a}{4\pi}\log\frac{x_0}{2k_{\min}}\frac{\Box^2}{x_0^2}\int[F_0(x_0-x_1)+F_1(x_0-x_1)]J_\mu(x_1)dx_1$$
$$+\frac{a}{4\pi}\frac{\Box^2}{x_0^2}\int\left[\frac{1}{2}F_0(x_0-x_1)+F_1(x_0-x_1)+\frac{1}{2}G(x_0-x_1)\right]J_\mu(x_1)dx_1$$
$$+\frac{a}{2\pi}c\frac{\partial}{\partial x_{0\nu}}\int F_0(x-x_1)m_{\mu\nu}(x_1)dx_1, \tag{38}$$

where

$$m_{\mu\nu}(x)=\frac{e}{2x_0}\bar\psi(x)\sigma_{\mu\nu}\psi(x),\quad \sigma_{\mu\nu}=\frac{1}{2i}(\gamma_\mu\gamma_\nu-\gamma_\nu\gamma_\mu), \tag{39}$$

and

$$G(x)=\int_0^1 dv(1+v^2)\frac{1}{(2\pi)^4}\int\frac{dp\,e^{ipx}\log(1+p^2(1-v^2)/4\varkappa_0^2)}{1+(p^2/4\varkappa_0^2)(1-v^2)}. \tag{40}$$

Thus the complete second order radiative correction to the Hamiltonian density for the elastic scattering of the electron is given by

$$H^{II}(x_0)=-ie\int dx_1\bar{\psi}(x_1)\Gamma'_\mu(x_0-x_1)\psi(x_1)A^e_\mu(x_0), \tag{41}$$

where

$$\begin{aligned}\Gamma'_\mu(x)=&\frac{\alpha}{4\pi}\gamma_\mu\log\frac{\varkappa_0}{2k_{\min}}\frac{\Box^2}{k_0^2}(F_0(x)+F_1(x))\\&+\frac{\alpha}{4\pi}\gamma_\mu\frac{\Box^2}{\varkappa_0^2}\left(\frac{1}{2}F_0(x)+\frac{1}{3}F_2(x)+\frac{1}{2}G(x)\right)\\&+\frac{\alpha}{2\pi}\left(\frac{-i}{2\varkappa_0}\right)\sigma_{\mu\nu}\frac{\partial}{\partial x_\nu}F_0(x).\end{aligned} \tag{42}$$

We shall now restrict the external potential to be that of a time independent scalar field and accordingly write

$$A^e_4(x_0)=iN(r). \tag{43}$$

The matrix element of the integral Hamiltonian for the elastic scattering for transitions from a state p to a state q in a static field $V(r)$ including the second order radiative corrections becomes

$$(p|H^{(0)}|q)=eV_{pq}\bar{u}(p)[\gamma_4+\Gamma_4(p-q)]u(q), \tag{44}$$

where $\Gamma_\mu(p-q)$ is the Fourier transform of $\Gamma'_\mu(x)$ defined by

$$\Gamma_\mu(p-q)=\int e^{-i(p-q)x}\Gamma'_\mu(x)\,dx, \tag{45}$$

$$\Gamma_4(p-q)=\frac{-\alpha}{4\pi}\gamma_4\left[4\lambda^2A(\lambda)+\frac{i}{\varkappa_0}F_0(\lambda)\vec{\gamma}\cdot(\vec{p}-\vec{q})\right], \tag{46}$$

where $A(\lambda)$, $F_0(\lambda)$ have been already defined by S. III and

$$V_{pq}=\int e^{-ik(p-q)}V(r)\,d\vec{r}, \tag{47}$$

the integral being extended over the surface $t=$constant.

We now proceed to evaluate the Hamiltonian density for the bremsstrahlung. Making use of the relation

$$S_F(p)=\int_{-\infty}^{\infty}dx\,e^{ipx}S_F(x)=\frac{-2i(i\gamma p-\varkappa_0)}{p^2+\varkappa_0^2}, \tag{48}$$

and putting

$$A_\nu(x)=A_\nu(k)\,e^{\pm ikz}, \tag{49}$$

where $\pm$ signs correspond to the emission and absorption of a quantum respectively, and performing the integration in (6) over the surface $t=$constant the matrix element of the integral Hamiltonian reduces to

$$(p|H^{(1)}|qk)=4\pi i\alpha\sqrt{\frac{\hbar c}{2k}}\,V_{p,\,q+k}\,e_\nu\bar{u}(p)\Big[\gamma_4\frac{i\gamma(q+k)-\varkappa_0}{2qk}\gamma_\nu$$
$$-\gamma_\nu\frac{i\gamma(p-k)-\varkappa_0}{2pk}\gamma_4\Big]u(q), \tag{50}$$

where we have put :—

$$A_\nu(k)=\sqrt{\frac{\hbar c}{2k}}\,e_\nu,\quad \psi(x)=u(q)e^{iqx},\quad \bar{\psi}(x)=\bar{u}(p)e^{-ipx}, \tag{51}$$

where e_ν is the unit vector in the direction of the polarisation of the emitted photon and

$$V_{p,\,q+k}=\int V(r)e^{-ix(p-q-k)}\,d\vec{r}\,. \tag{52}$$

For slowly moving particles the expressions (44) and (52) reduce to :

$$(p|H^{(0)}|q)=eV_{pq}\bar{u}(p)\gamma_4\Big[1-\frac{\alpha\delta}{4\pi}-\frac{(\vec{p}-\vec{q})^2}{\varkappa_0^2}-\frac{i\alpha}{4\pi\varkappa_0}\vec{\gamma}\cdot(\vec{p}-\vec{q})\Big]u(q), \tag{53}$$

and

$$(p|H^{(1)}|qk)=\frac{eV_{pq}C_1}{k^{3/2}}\bar{u}(p)\gamma_4\vec{e}\cdot(\vec{q}-\vec{p})u(q), \tag{54}$$

where

$$\delta=\frac{4}{3}\log\frac{\varkappa_0}{2k_{\min}}+\frac{17}{30},\quad C_1=\frac{e}{\varkappa_0\sqrt{2\hbar c}}. \tag{55}$$

§ 2. Radiation damping and the scattering cross-section

The covariant theory of radiation damping has already been discussed by Fukuda and Miyazima.[14] The S–matrix of Heisenberg describing the scattering processes is defined by

$$S=1+\sum_1^\infty\Big(\frac{-i}{\hbar c}\Big)^n\frac{1}{n!}\int_{-\infty}^{\infty}dx_1\ldots dx_n\,P(H^e(x_1),\ldots H^e(x_n)), \tag{56}$$

where P is the chronological ordering operator and $H^e(x_0)$ is the Hamiltonian for the external field, *including the radiative corrections*. The S–matrix is further expressed as

$$S=1-\frac{i}{\hbar c}R, \tag{57}$$

where R is proportional to amplitude of the scattered wave. Making the Cayley transformation :—

$$S=\frac{1-(i/2\hbar c)K}{1+(i/2\hbar c)K}, \tag{58}$$

where K is a Hermitian matrix, we obtain

$$R=K-\frac{i}{2\hbar c}KR, \tag{59}$$

which is the covariant generalisation of Heitler's equation for radiation damping. K has the following expansion :—

$$K=\sum_{n=1}^{\infty}\frac{1}{2^{n-1}}\left(\frac{-i}{\hbar c}\right)^{n-1}\int_{-\infty}^{\infty}dx_1\cdots dx_n\; H^e(x_1)\cdots H^e(x_n)\,\epsilon(\sigma_1,\sigma_2)\cdots\epsilon(\sigma_{n-1},\sigma_n), \qquad (60)$$

where $\epsilon(\sigma,\sigma')=+1$ if σ' antidates σ and -1 if σ' succeeds σ.

Since we are concerned with the scattering under the influence of a time-independent classical field we shall now specialise our discussion to the surface $t=$constant. It is then easily verified that

$$K=\int_{-\infty}^{\infty}dx\; H^e(x). \qquad (61)$$

Since the conservation of energy holds in the scattering process, we can conveniently express

$$R_{AB}=2\pi\delta(p_{0A}-p_{0B})\,V_{AB}, \quad K_{AB}=2\pi\delta(p_{0A}-p_{0B})\,H_{AB}, \qquad (62)$$

where p_{0A}, p_{0B} are the energies of the initial and final states A and B respectively and H_{AB} is proportional to the integral Hamiltonian. From (59), (61) and (62) we immediately obtain the familiar equation of radiation damping :—

$$V_{AB}=H_{AB}-\frac{i\pi\rho_C}{\hbar c}H_{AC}\,V_{CB}, \qquad (63)$$

where $\rho_C dE_C$ is the number of states C lying in the energy range E_C and E_C+dE_C.

It is to be emphasised that in the equation (63) the matrix elements include the radiative corrections upto any order of approximations, whereas in the corresponding equation of Heitler only the non-vanishing lowest orders of the matrix elements are retained. The differential cross-section is now given by

$$d\sigma_{AB}=\frac{2\pi}{\hbar v_A}|V_{AB}|^2\rho_B. \qquad (64)$$

§ 3. Radiative corrections to electron scattering

(A) *Without damping* (*Schwinger*) : We shall now investigate the elastic scattering of an electron in Coulomb field. We write (43) in the form

$$A_1^e(x_0)=\frac{ie\mathcal{Z}}{4\pi|\vec{r}|}, \qquad (65)$$

whence we obtain from (44)

$$(p|H^{(0)}|q)=\frac{e^2\mathcal{Z}}{|\vec{p}-\vec{q}|^2}\bar{u}(p\,[\gamma_4+\Gamma_4(p-q)]u(q). \qquad (66)$$

The cross-section for radiationless scattering is then given by

$$d\sigma_{AB}^{(0)}=\left|\frac{\vec{q}}{\vec{p}}\right|\frac{p_0q_0}{4\pi^2\hbar^2c^2}\cdot\frac{1}{2}\sum_{\text{Spin}}|H_{AB}^{(0)}|^2d\Omega_q$$

$$=2d\Omega_q\left[\frac{Z\alpha}{(\vec{p}-\vec{q})^2}\right]^2\frac{1}{4}\,\mathrm{Spur}\{(i\gamma p-\varkappa_0)(\gamma_4+\Gamma_4(q-p))(i\gamma q-\varkappa_0)(\gamma_4+\Gamma_4(p-q))\}, \tag{67}$$

which is the expression (2·64) of S. III.

For the scattering with the emission of radiation the integral Hamiltonian follows immediately from (50)

$$H_{AB}^{(1)}=4\pi\alpha\sqrt{\frac{\hbar c}{2k}}\cdot\frac{eZ}{|\vec{p}-\vec{q}-\vec{k}|^2}\cdot\bar{u}(p)\left[\frac{2(ep)-(e\gamma)(\gamma k)}{-2pk}\gamma_4\right.$$
$$\left.+\gamma_4\frac{2(eq)+(\gamma k)(e\gamma)}{2qk}\right]u(q). \tag{68}$$

The cross-section for radiative scattering is thus given by

$$d\sigma_{AB}^{(1)}=\frac{1}{2}\sum_{\text{Spin, pol}}|H_{AB}^{(1)}|^2\frac{2\pi}{\hbar^2c^2}\cdot\frac{|\vec{q}|p_0q_0}{|\vec{p}|}\cdot\frac{d^3\vec{k}}{(2\pi)^3}\cdot\frac{d\Omega_q}{(2\pi)^3}$$
$$=\frac{\pi^2}{\hbar c}\frac{|\vec{q}|}{|\vec{p}|}\frac{\alpha^2}{(2\pi)^5}\cdot\frac{e^2Z^2}{|\vec{p}-\vec{q}-\vec{k}|^4}\cdot\frac{d^3\vec{k}}{|\vec{k}|}\cdot d\Omega_q$$
$$\times\,\mathrm{Spur}\left\{(i\gamma p-\varkappa_0)\left(\frac{2(ep)-(e\gamma)(\gamma k)}{-2pk}\gamma_4+\gamma_4\frac{2(eq)+(\gamma k)(e\gamma)}{2qk}\right)\right.$$
$$\left.\times\,(i\gamma q-\varkappa_0)\left(\gamma_4\frac{2(ep)-(\gamma k)(e\gamma)}{-2pk}+\frac{2(eq)+(e\gamma)(\gamma k)}{2qk}\gamma_4\right)\right\}. \tag{69}$$

We have thereby utilised the relation

$$\sum_{\text{Spin}}u_\alpha(p)\bar{u}_\beta(p)=-\frac{1}{2p_0}(i\gamma p-\varkappa_0)_{\alpha\beta}. \tag{70}$$

The expression (69) agrees with the lowest order cross-section for bremsstrahlung obtained by Heitler.[15] It is to be observed that for the essentially elastic scattering in which a small fraction of the electron kinetic energy is radiated we obtain from (69)

$$d\sigma_{AB}^{(1)}=\frac{\alpha}{2\pi^2}\left(\frac{Z\alpha}{2p_0\beta^2}\mathrm{cosec}^2\theta/2\right)^2(1-\beta^2\sin^2\theta/2)\frac{d^3\vec{k}}{2|\vec{k}|}\cdot d\Omega_q\sum_{\text{pol}}\left(\frac{eq}{qk}-\frac{ep}{pk}\right)^2, \tag{71}$$

which is equivalent to expression (2·80) of S. III. It has been shown by Schwinger (S. III) that in the non-relativistic approximation the infra-red divergence contained in (67) is cancelled by the similar one arising from (69).

(B) *With damping* (*Bethe and Oppenheimer*): We are now in a position to evaluate the effect of the radiation damping on the scattering of the electron. Following Bethe and Oppenheimer we shall assume that the matrix elements of the scattering potential energy $V_1=eV_{pq}$ do not depend on the directions of the vectors $\vec{p}$ and $\vec{q}$ but make no restrictions on its magnitude. We shall further neglect the higher order effects such as the emission of two quanta or the scattering of quanta.

The equations of radiation damping for transitions without radiation and for scattering with emission of radiation are obtained from (63) and given respectively by

$$(q|U|p)=(q|H|p)-\frac{i\pi p^2}{c\hbar(2\pi)^3}\int d\Omega'\Big[(q|H|p')(p'|U|p)$$
$$+\frac{d^3\vec{k}}{(2\pi)^3}(q|H|p'k)(p'k|U|p), \tag{72}$$

$$(p'k|U|p)=(p'k|H|p)-\frac{i\pi}{c\hbar}\cdot\frac{p^2}{(2\pi)^3}\int d\Omega''[(p'k|H|p''k)(p''k|U|p)$$
$$+(p'k|H|p'')(p''|U|p)]. \tag{73}$$

$\vec{p}$, $\vec{q}$, $\vec{p}'$, $\vec{p}''$ denote the momenta of the electron, p is the absolute value of the momentum which is the same for all states, the integral $d\Omega'$ is over all directions of $\vec{p}'$ and the integral $d^3\vec{k}$ is over magnitude, direction and polarisation of the light quantum.

To solve the equations (72) and (73) we assume

$$(q|U|p)=\bar{u}(q)\gamma_4[A_1+(\vec{\gamma}\cdot\vec{q})A_2+(\vec{\gamma}\cdot\vec{p})A_3+(\vec{\gamma}\cdot\vec{q})(\vec{\gamma}\cdot\vec{p})A_4+(\vec{p}\cdot\vec{q})A_5]u(p), \tag{74}$$

$$(qk|U|p)=-\frac{1}{k^{3/2}}\bar{u}(q)\gamma_4[B_1(\vec{e}\cdot\vec{q})+B_2(\vec{e}\cdot\vec{p})+(\vec{e}\cdot\vec{\gamma})B_3+(\vec{e}\cdot\vec{\gamma})(\vec{\gamma}\cdot\vec{p})B_4$$
$$+(\vec{e}\cdot\vec{q})(\vec{\gamma}\cdot\vec{p})B_5]u(p). \tag{75}$$

It is to be noted that the coefficients A's and B's are matrices which involve γ_4 only and not the other γ's.

We now substitute (74) and (75) in (73) and sum over the spins in the intermediate states and integrate over the angles. We thereby remember the relations (70) and note that in the terms containing an odd number of factors involving $\vec{p}'$ vanish on integration and that

$$\int(\vec{a}\cdot\vec{p}')(\vec{b}\cdot\vec{p}')d\Omega'=\frac{4\pi}{3}(\vec{a}\cdot\vec{b})p^2. \tag{76}$$

Equating the coefficients of $(\vec{e}\cdot\vec{q})$, $(\vec{e}\cdot\vec{p})$ etc. on both sides of the resulting equation we obtain

$$B_1=V_1C_1-iW_1C_1((p_0+\varkappa_0\gamma_4)A_1+ip^2\gamma_4A_2),$$
$$B_2=-V_1C_1-iW_1(p_0+\varkappa_0\gamma_4)\Big(B_2-\frac{1}{3}p^2C_1A_5\Big),$$
$$B_3=-iW_1(p_0-\varkappa_0\gamma_4)\Big(B_3-\frac{1}{3}p^2A_2^2C_1\Big)-\frac{W_1p^2}{3}\gamma_4(B_1-C_1A_1),$$
$$B_4=-iW_1(p_0+\varkappa_0\gamma_4)\Big(B_4-\frac{1}{3}C_1p^2A_4\Big)+\frac{W_1p^2}{3}\gamma_4(B_5-C_1A_3),$$
$$B_5=-iW_1C_1(p_0-\varkappa_0\gamma_4)A_3-W_1C_1p^2\gamma_4\Big(A_4+\frac{1}{3}A_5\Big), \tag{77}$$

where

$$V_1=eV_{pq}, \quad W_1=\frac{V_1p}{4\pi\hbar c}. \tag{77a}$$

Similarly to solve (72) we substitute (74) and (75) in it and note that the photons $\vec{k}$ emitted are virtual photons and the integration is over $d^3\vec{k}=k^2dk\,d\Omega_k$. Performing the integrations and using the abbreviations

$$\eta=\frac{\alpha}{4\pi}\delta\frac{2p^2}{\varkappa_0^2},\quad R=\frac{C_1^2p^2}{3\pi^2}\log\frac{p^2}{2\varkappa_0 k_{\min}},\tag{78}$$

and introducing

$$\zeta=\eta-R=\frac{2\alpha p^2}{3\pi\varkappa_0^2}\left[\frac{17}{40}-\log\frac{p^2}{\varkappa_0^2}\right],\tag{79}$$

which is finite and free from $k_{\min}$, we can easily determine the coefficients A's by comparing their coefficients on both sides of the equations. By retaining only the terms upto the order of α and p^2 in matrix elements (74) and (75) we obtain finally the following solution for the amplitudes:

$$A_1=\frac{V_1(1-\eta)}{1+iW_1(p_0+\varkappa_0\gamma_4)}+\frac{V_1}{[1+iW_1(p_0+\varkappa_0\gamma_4)]^2}\left\{iW_1\zeta(p_0+\varkappa_0\gamma_4)-\frac{iW_1\alpha p^2\gamma_4}{2\varkappa_0\pi}\right\},$$

$$A_2=\frac{-iV_1\alpha/(4\pi\varkappa_0)}{1+iW_1(p_0+\varkappa_0\gamma_4)},\quad A_3=\frac{iV_1\alpha}{4\pi\varkappa_0}\times\frac{1+iW(p_0+\varkappa_0\gamma_4)}{1+2iW_1p_0},$$

$$A_4\approx 0,\quad A_5=-\frac{V_1}{p^2}\cdot\frac{\eta+iW_1\zeta(p_0+\varkappa_0\gamma_4)}{1+iW_1(p_0+\varkappa_0\gamma_4)},$$

$$B_1=-B_2=\frac{V_1C_1}{1+iW_1(p_0+\varkappa_0\gamma_4)},\quad B_3=B_4=B_5=0.\tag{80}$$

Substituting these expressions in (74) and (75) we get the matrix elements $(q|U|p)$ and $(qk|U|p)$ up to the order of α; the cross-section for radiationless scattering is then given by

$$\frac{d\sigma_0}{d\Omega_q}=\frac{p_0^2}{4\pi^2\hbar^2c^2}\frac{1}{2}\sum_{\text{Spin}}|(p|U|q)|^2.\tag{81}$$

The cross-section for scattering with the emission of radiation is given by

$$\frac{d\sigma_1}{d\Omega_q}=\frac{p_0^2}{c^2\hbar^2}\int_{k_{\min}}^{(p^2/2\varkappa_0)}k^2dk\frac{1}{2}\sum_{\text{Spin, pol}}|(p|U|qk)|^2\frac{d\Omega_k}{(2\pi)^5}.\tag{82}$$

Using formula (70) for the annihilation operator and evaluating the spurs, we get

$$d\sigma_0=\lambda\bar{\lambda}^2W^2\left[\frac{1+(\vec{p}\cdot\vec{q}+p^2)/2\varkappa_0^2}{1+W^2}-\frac{(1-\vec{p}\cdot\vec{q}/p^2)(2\eta-\alpha p^2/2\pi\varkappa_0^2)}{1+W^2}\right.$$

$$\left.+\frac{2W^2}{(1+W^2)^2}\left(\zeta-\frac{p^2\alpha}{4\pi\varkappa_0^2}-\frac{p^2}{4\varkappa_0^2}\right)\right]d\Omega_q,\tag{83}$$

and

$$d\sigma_1=\frac{2\lambda^2W^2R}{1+W^2}\left(1-\frac{\vec{p}\cdot\vec{q}}{p^2}\right)d\Omega_q,\tag{84}$$

where following Bethe and Oppenheimer, we have put

$$W=2\varkappa_0 W_1\,, \quad \lambda=\frac{1}{p}\,. \tag{85}$$

Adding the two cross sections (83) and (84) and noting the relation (79) we get finally,

$$d\sigma=W^2\lambda^2\Big[\frac{1+(\vec{p}\cdot\vec{q}+p^2)/2\varkappa_0^2}{1+W^2}+\frac{(1-\vec{p}\cdot\vec{q}/p^2)(p^2u/2\pi\varkappa_0^2-2\zeta)}{1+W^2}$$
$$+\frac{2W^2}{(1+W^2)^2}\Big(\zeta-\frac{p^2u}{4\pi\varkappa_0^2}-\frac{p^2}{4\varkappa_0^2}\Big)\Big]d\Omega_q\,. \tag{86}$$

The expression (86) is thus entirely free from the infra-red divergences. It is to be observed that the infra-red catastrophe involved in the scattering with emission of radiation given by (84) is now exactly compensated by the corresponding term due to the second order radiative corrections, occuring in the radiationless scattering (83).

References

1) F. Bloch and A. Nordsieck, Phys. Rev. **52** (1937), 54.
2) W. Pauli and M. Fierz, Nuovo Cimento **15** (1938), 167.
3) W. Braunbek and E. Weinmann, ZS. f. Phys. **110** (1938), 360.
4) S. M. Dancoff, Phys. Rev. **55** (1939), 959.
5) H. W. Lewis, Phys. Rev. **73** (1948), 173.
6) S. T. Epstein, Phys. Rev. **73** (1948), 177.
7) H. A. Bethe and J. R. Oppenheimer, Phys. Rev. **70** (1946), 451.
8) W. Heitler, Proc. Camb. Phil. Soc. **37** (1941) 291.
W. Heitler and H. W. Peng, Proc. Camb. Phil. Soc. **38** (1942), 296.
H. A. Wilson, Proc. Camb. Phil. Soc. **37** (1941), 301.
9) R. C. Majumdar, and B. P. Nigam, Proc. International Conference on Elementary Particles, p. 173, (1950).
W. Heitler and S. T. Ma, Phil. Mag. **40** (1949), 651.
10) W. Pauli, International Physics Conference at Cambridge, July 1946, *Meson Theory of Nuclear Forces*, New York, 1946.
11) S. Tomonaga, Prog. Theor. Phys. **1** (1946) 27 and a series of subsequent papers.
12) J. Schwinger, Phys. Rev. **74** (1948), 1439, I; Phys. Rev. **75** (1949), 651, II; Phys. Rev. **76** (1949), 790, III. This paper is referred in the Text as S. III.
13) R. Karplus and N. M. Kroll, Phys. Rev. **77** (1950), 536.
14) N. Fukuda and T. Miyazima, Prog. Theor. Phys. **5** (1950), 849.
15) W. Heitler, *The Quantum Theory of Radiation*, 1944.

Letters to the Editor

On the Interaction Representation

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In order to treat the interacting system in relativistically covariant manner, it is appropriate to use the interaction representation which was founded in 1946 by Tomonaga[1]. In the theory of this representation, the dominant role is played by the covariant commutation relation of the free field based on the method of Jordan-Pauli[2] and the interaction Hamiltonian determining the motion of the state vector and the unitary transformation which connects the free equation of motion and one in the Heisenberg representation.

With regard to the interaction Hamiltonian, however, there has been the erroneous argument that it should be determined by the integrability condition of the Tomonaga equation (i.e. the Schrödinger equation in the interaction representation)[3][4]. But this condition does not uniquely determine the correct interaction Hamiltonian and only one of those which satisfy the condition corresponds to the unitary transformation connecting the two equations of motion in both representations. Moreover, in the formalism so far developed, the general and simple method to determine the covariant commutation relation for the free field with the arbitrary spin has not been found.

In this note, the method to obtain the covariant commutation relation of the free field and the correct interaction Hamiltonian and the general formalism of the interaction representation based on those methods are briefly discussed.

(I) We write the respective equation of motion in the Heisenberg and the interaction representations as follows:

$$A_{\alpha\beta}(\partial)\underline{Q_\beta}(x)=D_\alpha \underline{j_\alpha}:_\alpha(x), \tag{1}$$

$$A_{\alpha\beta}(\partial)Q_\beta(x)=0, \tag{2}*$$

where

$$\left.\begin{aligned} &D_\alpha\equiv D_{\mu_1\cdots\mu_n}=(-1)^n\partial_{\mu_1}\cdots\partial_{\mu_n},\\ &\underline{j_\alpha}:_\alpha\equiv \underline{j_\alpha}:_{\mu_1\cdots\mu_n}=\partial L/\partial Q_\alpha:_{\mu_1\cdots\mu_n},\\ &Q_\alpha:_{\mu_1\cdots\mu_n}=\partial_{\mu_1}\cdots\partial_{\mu_n}Q_\alpha, \end{aligned}\right\} \tag{3}$$

and the L is the interaction Lagrangian. When (2) is compatible with the equations of the harmonic oscillator,

$$(\Box-\varkappa^2)Q_\alpha(x)=0.$$

We can prove that the commutation relation is given by

$$[Q_\alpha(x),\ Q_\beta(x')]=iR_{\alpha\beta}(\partial)\Delta(x-x') \tag{4}$$

by use of $R_{\alpha\beta}(\partial)$ which is the derivation operator satisfying the relation

$$A_{\alpha\beta}(\partial)R_{\beta\gamma}(\partial)=(\Box-\varkappa^2)\delta_{\alpha\gamma}. \tag{5}$$

Using (5) and the fact that the maximum degree of the differentiation in $R_{\alpha\beta}(\partial)$ is $2s$ for the field with spin s (mass $\varkappa\neq0$), we can obtain $R_{\alpha\beta}(\partial)$ for the arbitrary field. (5) is also the important relation between the Green function and the covariant commutation relation.

(II) As to the interaction Hamiltonian $H(x;n)$ and the unitary transformation $U(\sigma)$ which connects the Heisenberg- and the interaction-representations, we have the relation

$$i\frac{\delta U(\sigma)}{\delta\sigma(x)}=H(x;n)U(\sigma)=U(\sigma)H(x,\sigma;n)|_{x/\sigma}. \tag{6}**$$

$H(x;n)$ is obtained by means of the *fundamental relation of our formalism*

$$[Q_\alpha(x,\sigma),\ H(x'/\sigma;n)]=iR_{\alpha\beta}(\partial)D_\alpha\Delta(x-x')\underline{j_\beta}:_\alpha(x'), \tag{7}$$

where $Q_\alpha(x,\sigma)$ is the auxiliary operator which satisfies the free equation (2) and the same commutation relation as (4) for the fixed surface σ and

$$Q_\alpha(x,\sigma)=U^{-1}(\sigma)Q_\alpha(x)U(\sigma). \tag{8}$$

Since the Heisenberg operator $\underline{Q_\alpha}(x)$ has the relation

$$\begin{aligned}\underline{Q_\alpha}(x)=&Q_\alpha(x/\sigma)\\&+\frac{1}{2}\int[D_\alpha R_{\alpha\beta}(\partial),\varepsilon(x-x')]\Delta(x-x')\\&\times\underline{j_\beta}:_\alpha(x')d\lambda'\end{aligned} \tag{9}***$$

with the above $Q_\alpha(x,\sigma)$, the right hand side of (7) is expressed successively by $Q_\alpha(x/\sigma)$ and $H(x/\sigma;n)$ is determined. Moreover we can prove that the interaction Hamiltonian thus obtained satisfies the integrability condition of the Tomonaga equation.

(III) Using the interaction Hamiltonian previously obtained, the energy-momentum four vector is defined as follows:

$$\underline{T}_\mu = U^{-1}(\sigma)\int_\sigma \{T_{\mu\nu}{}^0(x') - \delta_{\mu\nu} H(x'; n)\}\, d\sigma_\nu' U(\sigma), \tag{10}$$

where $T_{\mu\nu}{}^0(x)$ is the canonical energy-momentum tensor of the free field. In fact, taking into account the integrability condition and the fact that $\underline{Q}_\alpha(x)$ is the point function, we can show that $\underline{T}_\mu$ satisfies the continuity equation and is the time space displacement operator in the Heisenberg representation.

$R_{\alpha\beta}(\partial)$ has generally the term proportional to $(\Box - \varkappa^2)$ which does not contribute to the commutation relation (4), but this term plays the important role as the Green function and gives the term independent of the normal in $\{H(x; n) - (-L(x))\}$. This is the very reason why the integrability condition cannot determine uniquely the interaction Hamiltonian. According to our theory, it is known that if we use $\Delta_F{}^*$ as Koba[4], the terms proportional to $(\Box - \varkappa^2)$ in the Green function are discarded and the wrong result is obtained.

The rule of the automatical cancellation of the normal-dependent terms in the S-matrix is not the $\Delta_F{}^*$-method of Koba but must be improved as follows:

a) $H(x; n)$ is replaced by $-L(x)$,

b) $\langle P(M(\partial) Q_\alpha(x),\ N(\partial') Q_\beta(x'))\rangle_0$ is replaced by

$$\frac{1}{2} R_{\alpha\beta}(\partial) M(\partial) N(\partial') \Delta_F(x - x'),$$

where $M(\partial)$ and $N(\partial')$ are the arbitrary derivation operators. Hereupon, we can obtain the S-matrix independent of the normal of the surface and compatible with the equation of motion.

In addition, the same argument holds true in the non-local action and we can also see on the basis of (5) the intimate connection between the non-local action and the non-local interaction. The detail will appear in later occasion.

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*) In this paper, we denote the field quantity in Heisenberg representation by the under-line and the suffix α labels the different types of the field as well as the components of each field.

**) x/σ means x on the surface σ and $H(x, \sigma; n)$ is the functional of $Q_\alpha(x, \sigma)$ having the same form as the functional $H(x; n)$ of $Q_\alpha(x)$.

***) We must bear in mind the fact that $\underline{Q}_\alpha(x)$ does not always coincide $Q_\alpha(x/\sigma)$ if the suffix α labels the constraint variable and one of such examples is seen in the fourth component of the vector meson field.

1) S. Tomonaga, Prog. Theor. Phys. **1** (1946), 27.
2) P. Jordan and W. Pauli, ZS. f. Phys. **47** (1928), 151.
3) S. Kanesawa and Z. Koba, Prog. Theor. Phys. **4** (1949), 297.
4) Z. Koba, Prog. Theor. Phys. **5** (1950), 696.

Tomonaga Approximation in Meson Theory

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Recent study of the meson theory seems to have much success. Both perturbation theory including the higher order radiative corrections and strong coupling theory succeed to describe the nature of meson-nucleon interaction at least qualitatively and sometimes quantitatively. Inspite of the successes, we may ask whether the methods of calculations in both theories are adapted to the problem or not. It is probable that the coupling of mesons with nucleons is rather large but not so extremely, i.e. lies in the so-called "intermediate" region. Tomonaga proposed one method of approximation applicable in this region, which is based on Ritz's variation principle. Moreover, he showed that the result agrees in the two limiting cases with those from the conventional theories, i.e. in the weak coupling limit with that of the usual perturbation theory and in the strong coupling limit with that of the strong coupling theory. It may be worthy of extending his theory and comparing the results with those of the conventional theories for the various types of the mesons. Here Tomonaga approximation is applied to the scalar and pseudoscalar mesons, neutral, charged and symmetrical.

To solve the Schroedinger equation

$$H\Psi = E\Psi, \tag{1}$$

we treat all the problem in Fock space. Ψ is expanded as follows:

$$\Psi=\sum F(k_1, k_2, \cdots, k_n)|k_1, k_2, \cdots, k_n\rangle, \quad (2)$$

here k's are the observables specifying the states of the mesons, and the summation is taken over n and k's. Ket $|k_1, k_2, \cdots, k_n\rangle$ satisfies the following relations

$$\langle k_1', k'_2, \cdots, k'_m|k_1, k_2 \cdots, k_n\rangle \quad (3)$$
$$=\delta_{m,n}\,\delta_{k_1 k_1'}\,\delta_{k_2 k_2'}\cdots\delta_{k_m k_n'},$$

$$a^*(k)|k_1, k_2, \cdots, k_n\rangle=(n+1)^{-1/2}|k_1, k_2, \cdots, k_n, k\rangle, \quad (4)$$

$$a(k)|k_1, k_2, \cdots, k_n\rangle=n^{1/2}\sum_{r=1}^{n} \times|k_1, \cdots, k_{r-1}, k_{r+1}\cdots k_n\rangle\,\delta_{k,k_r}. \quad (5)$$

Our problem is to find $F(k_1, k_2, \cdots, k_n)$ under certain boundary condition. The essential point of the Tomonaga approximation is to assume the form of the function F as

$$F(k_1, k_2, \cdots, k_n)=c_n f(k_1) f(k_2)\cdots f(k_n), \quad (6)$$

where c_n and $f(k)$ are to be determined by the variation principle

$$\delta(\Psi, H\Psi)=0 \qquad \text{under } (\Psi, \Psi)=1. \quad (7)$$

For the neutral scalar meson theory total Hamiltonian is

$$H=\sum N_k\omega_k+\sum[a(k)+a^*(k)]\,g(k), \quad (8)$$

where $g(k)=g/(2\omega_k V)^{1/2}$. In convenience we write Ψ as

$$\Psi=N\sum_{n=0}^{\infty}\frac{c_n}{\sqrt{n!}}\sum_{k_i} f(k_1)f(k_2)\cdots f(k_n)|k_1, k_2, \cdots, k_n\rangle. \quad (9)$$

variation principle gives a set of the simultaneous equations

$$EWc_n=E_s Wc_{n+1}+nE_s c_{n-1}+n\varepsilon c_n, \quad (n=0, 1, 2, \cdots), \quad (10)$$

where $W=\sum f(k)^2$, $E_s=\sum f(k)\,g(k)$ and $\varepsilon=\sum\times f(k)^2\,\omega_k$. Equations (10) have the physically meaningful solutions for the special values of E.

$$E=-E_s^2/\varepsilon+\mu(\varepsilon/W), \quad \mu=0, 1, 2, \cdots. \quad (11)$$

Variation of (11) determines the function $f(k)$.

Now we shall discuss the boundary condition. Firstly we consider the limiting case $g\to 0$. We postulate that in this limit the mesons do not interact with the nucleons and the Ψ contains a single term $c_0|\,\rangle$ only. This leads the vanishing value of E, and in (11) μ must be zero. In this case $c's=1$, $f(k)=-g(k)/\omega_k$ and $E=-\varepsilon$ hold. However, under other B.C., for example if we refer (9) only in the strong coupling limit, non-zero value of μ are not excluded.

Thus, our problem strongly depends on the B.C. considered. In the following we consider the B.C. in the weak coupling limit, and do not refer to the strong coupling limit. (Detailed discussions will be given in the complete paper.)

For charged theory, the Ψ will be written for charge 1 state as

$$\Psi=N\sum\frac{a_n}{\sqrt{n!\,n!}}\sum f(k_1^+)\cdots f(k_n^-)|k_1^+, \cdots, k_n^+, k_1^-, \cdots, k_n^-\rangle$$
$$+N\sum\frac{b_n}{\sqrt{n!\,(n+1)!}}\sum f(k_1^+)\cdots f(k_n^-)|k_1^+, \cdots, k_{n+1}^+, k_1^-, \cdots, k_n^-\rangle. \quad (12)$$

Variation principle gives

$$\begin{aligned}&-a_n(EW-2n\varepsilon)+WE_s b_n+nE_s b_{n-1}=0,\\ &-b_n(EW-(2n+1)\varepsilon)+WE_s a_{n+1}\\ &\qquad+(n+1)E_s a_n=0.\end{aligned} \quad (13)$$

For simplicity we assume that $f(k^+)=f(k^-)$. (This restriction can be removed easily.) General discussion of (13) leads that there are eigenvalues of $E_{m,\mu}$, where m is related to the total charge. It has been interpreted that the state corresponding to the value

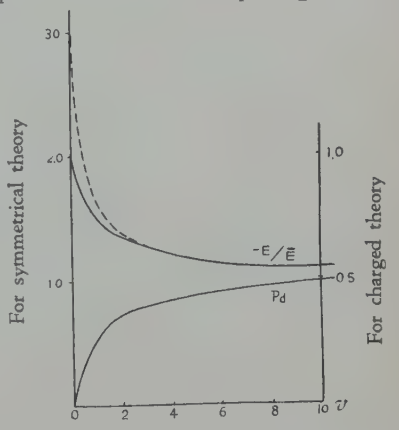

Fig. 1. Energy E and the dissociation probability P_d, where

$$\bar{E}=\sum g(k)^2/\omega(k)$$

Full curve for charged theory and the dotted curve for symmetrical theory.

of $m=1/2$ is proton state and those corresponding to the values of $m=\pm 3/2, \pm 5/2, \cdots$ are the isobar states. The B.C. argument along the same line as above, we take up only $E_{\pm 1/2,0}$ here.

Now we must resort in so tedious numerical calculations to solve (13), that we sssume a's and b's are unity and then determine $f(k)$. Fig. 1 shows the energy E and the dissociation probability P_d vs. $v=\sum_{\mathcal{S}}(k)^2/\omega^2$, in which the dotted line corresponds to the symmetrical theory calculated in the same assumption.

Next we consider the one meson problem. For the neutral scalar mesons, the problem is exactly soluble by the transformation of H_0,

$$\Psi=\exp(-W/2)\sum_{m=0}\frac{1}{\sqrt{m!}}\sum_{k_i\neq k_0} f(k_1)\, f(k_2)\cdots f(k_m)$$
$$\times\sum_{n=0}\frac{1}{\sqrt{n!}} f(k_0)^n (n/f(k_0)-f(k_0))$$
$$\times|k_1, k_2, \cdots, k_m;\ n(k_0)\rangle. \qquad (14)$$

Here ket $|k_1, \cdots, k_m;\ n(k_0)\rangle$ satisfies the following relations

$$a^*(k^0)|k_1, \cdots, k_m;\ n(k_0)\rangle = \sqrt{n+1}\,|k_1, \cdots, k_m;\ n+1(k_0)\rangle,$$
$$a(k_0)|k_1, \cdots, k_m;\ n(k_0)\rangle = \sqrt{n}\,|k_1, \cdots, k_m;\ n-1(k_0)\rangle. \qquad (15)$$

We can see that corresponding to the presence of one meson with momentum k_0 the factor $f(k_0)^n(n/f(k_0)-f(k_0))$ appears in F. Applying this idea to the charged and symmetrical theory we get the Ψ, which satisfies the B.C. that in the limit $g\to 0$ only one meson with momentum k_0 and the given charge and one nucleon, not interacting each other, are present. Comparing with the one nucleon problem, a's and b's satisfy the same equations (13), and the energy $E'=E+\omega(k_0)$ and $f(k)$'s are unchanged except $f(k_0)$, in the zero-th order of the volume V.

For the pseudoscalar meson theory we propose to apply the same approximation (9) with a slight care. $g(k)$'s include the spin $\boldsymbol{\sigma}$, so that the $f(k)$'s may also include the $\boldsymbol{\sigma}$. Then (9) is replaced by

$$\frac{1}{n!}\sum_{P} f(k_1)\, f(k_2)\cdots f(k_n). \qquad (16)$$

Notation $\sum_P$ means that the summation is taken over all the permutations of the order of the factors $f(k_1)$, $f(k_2), \cdots, f(k_n)$. After a slightly complicated calculation we find that the eigenvalue E is labelled by two parameters, one is related to the total spin of the system and the other is μ. We proceed the analogous discussion on the B.C. problem. Fig. 2 shows the energy and P_d for the neutral and the charged theory.

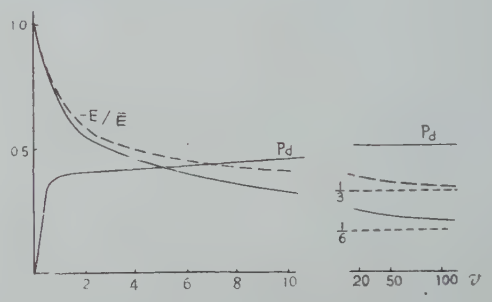

Fig. 2. Energy E and the dissociation probability P_d for pseudoscalar theory. Full curve for charged theory and the dotted curve for neutral theory.

From the figures we could see that the energy E is identical in the two limiting cases with those of the conventional theories for all types of the meson field, especially also in the pseudoscalar cases. Thus it may be concluded that Tomonaga approximation and its pseudoscalar extension will be a good approximation for the energy problem.

Anomalous magnetic moment of the nucleon is calculated by using of the one nucleon Ψ and the photomeson production cross section by the one nucleon and one meson Ψ. The complete paper including such problems will be published in this journal.

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On the Inelastic Collision between Molecules, II

— *Rotational Transition of H_2-molecule in the Collision with another H_2-molecule* —

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In this paper we consider the rotational transition of H_2-molecule in the collision with another H_2-molecule. The general derivation of the cross section and an example of the numerical calculation by a simplified method of approximation are presented. The result is compared with experimental value of the transition rate in H_2 gas obtained from the anomalous dispersion of the supersonic wave. The agreement of the calculated and the experimental rates is found to be within factor 2, and this is better than is expected under the accuracy of the approximation employed and also under the present situation concerning the knowledge of the intermolecular force.

§ 1. Introduction

In the previous paper[1] we inferred that the method of distorted wave is adequate to treat the energy transfer between the vibrational and the translational degrees of freedom in the molecular collision. The energy transfer between the rotational and the translational degrees of freedom has been treated similarly by the method of distorted wave. In this field, the calculation for the H_2-molecule is especially interesting because its result can be compared with the experimental data obtained recently from the anomalous dispersion of the supersonic wave in the hydrogen gas.[2] Such calculation was performed many years ago by Roy and Rose.[3] However, their calculation was restricted to estimating the lower limit of the cross section, since their aim was to explain the negative result of the earlier experiment.

In § 2, we formulate the problem and derive formally the cross section for the transition considered. It must be noted that the intermolecular force is essentially different from the spherically symmetric one. In our present case, the orbital angular momentum $\boldsymbol{j}$ of the relative motion of the two molecules is not a constant of motion. Instead, the total angular momentum $\boldsymbol{J}$ is a constant of motion, which is the vector sum of the orbital angular momentum $\boldsymbol{j}$ and the rotational angular momenta of the two molecules, and which defines the rotational state of the whole system. Curtiss, Hirschfelder and Adler[4][5] showed that it was possible to separate the rotational coordinate from the n-particle Schrödinger equation, and applies the resulting equation to the scattering of atoms from diatomic molecules. Following their procedure, one considers the state having definite J and sums up the final result over J. We may also apply their procedure to our system consisting of two diatomic molecules. But, in this paper, we need not proceed in this way, because

our treatment is based on the assumption that the coupling between the translational and the rotational degrees of freedom is so small, that the method of distorted wave can be used.

In § 3, we calculate the matrix elements of the interaction potential sandwiched by the angular part of the wave functions, assuming a simple form for the potential.

In § 4, we enumerate various methods of approximation for the solution of the radial equation, and in § 5, we apply the most simple method of them to calculate the rate of the rotational transition in the hydrogen gas. The resulting rate is compared with the experimental data mentioned above[2] and the agreement within factor 2 is obtained in spite of the simplified method employed.

§ 2. General theory for the derivation of the total cross section

In the following, we consider the collision of two diatomic molecules with each other. Both molecules are assumed to be in the vibrationally ground state and the nuclear distances inside each molecule are assumed to be constant.

Several notations must be defined before proceeding further. The center-of-gravity coordinate system is used throughout. Thus the translational motion of the system as a whole has been separated out.

$\boldsymbol{R}$ is a vector connecting the centers-of-gravity of two colliding molecules. θ_i, φ_i $(i=1, 2)$ represent the orientation of the i-th molecule in the space. χ_i, ψ_i represent the orientation relative to the vector $\boldsymbol{R}$.

$$\mu=(m_1+m_2)(m_3+m_4)/(m_1+m_2+m_3+m_4),$$

$$M_1=m_1m_2/(m_1+m_2), \quad M_2=m_3m_4/(m_3+m_4),$$

where m_k is the mass of the k-th atom. (see fig. 1). The atomic units are used throughout this paper.

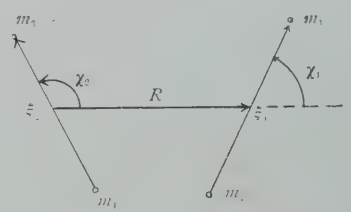

Fig. 1

The Schrödinger equation for our system is

$$\{\Delta/2\mu-H+W-V(R, \chi_1, \chi_2, \psi_1-\psi_2)\}\Psi=0, \tag{1}$$

where H is the sum of the Hamiltonians for the two rotators and W is the total energy of the system. The wave function may be expanded as*)

$$\Psi=\sum_{l_1m_1l_2m_2} f_{l_1m_1l_2m_2}(\boldsymbol{R})\, Y_{l_1m_1}(\theta_1, \varphi_1)\, Y_{l_2m_2}(\theta_2, \varphi_2). \tag{2}$$

Then we find that

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* The atomic mass does not appear explicitly hereafter. Thus m_1, m_2 always represent the quantum numbers in the following. Y_{lm} are the normalized spherical harmonics from which we get the eigenfunctions of the operator H as follows:

$$HY_{l_1m_1}(\theta_1, \varphi_1)\, Y_{l_2m_2}(\theta_2, \varphi_2)=\left(\frac{l_1(l_1+1)}{2M_1\xi_1^2}+\frac{l_2(l_2+1)}{2M_2\xi_2^2}\right) Y_{l_1m_1}(\theta_1, \varphi_1)\, Y_{l_2m_2}(\theta_2, \varphi_2).$$

$$(\Delta^2+k_{l_1l_2}{}^2)f_{l_1m_1l_2m_2}=2\mu\sum_{l_1'm_1'l_2'm_2'}(l_1m_1l_2m_2|V|l_1'm_1'l_2'm_2')f_{l_1'm_1'l_2'm_2'}, \tag{3}$$

where

$$k_{l_1l_2}{}^2/2\mu=W-l_1(l_1+1)/2M_1\xi_1{}^2-l_2(l_2+1)/2M_2\xi_2{}^2 \tag{3a}$$

and

$$(l_1m_1l_2m_2|V|l_1'm_1'l_2'm_2')$$
$$=\int Y_{l_1m_1}^{*}(\theta_1,\varphi_1)\,Y_{l_2m_2}^{*}(\theta_2,\varphi_2)\,V\,Y_{l_1'm_1'}(\theta_1,\varphi_1)\,Y_{l_2'm_2'}(\theta_2,\varphi_2)\,d\Omega_1\,d\Omega_2, \tag{3b}$$
$$(d\Omega=\sin\theta\,d\theta\,d\varphi).$$

If f's are further expanded in the form

$$f_{l_1m_1l_2m_2}(\boldsymbol{R})=\sum_{j,m}(2j+1)^{1/2}\{g^{jm}_{l_1m_1l_2m_2}(R)/R\}\,Y_{jm}(\Theta,\Phi), \tag{4a}$$

we get

$$\left\{\frac{d^2}{dR^2}-\frac{j(j+1)}{R^2}+k_{l_1l_2}{}^2\right\}g^{jm}_{l_1m_1l_2m_2}(R)$$
$$=2\mu\sum_{l_1'm_1'l_2'm_2'j'm'}(l_1m_1l_2m_2jm|V|l_1'm_1'l_2'm_2'j'm')\,g^{j'm'}_{l_1'm_1'l_2'm_2'}(R), \tag{4}$$

where

$$(l_1m_1l_2m_2jm|V|l_1'm_1'l_2'm_2'j'm')$$
$$=(2j'+1/2j+1)^{1/2}\int Y_{jm}^{*}(\Theta,\Phi)\,(l_1m_1l_2m_2|V|l_1'm_1'l_2'm_2')\,Y_{j'm'}(\Theta,\Phi)\,d\Omega. \tag{4b}$$

Let us now solve the equation (4) by the approximate method of distorted wave. In the following the abbreviation L stands for a set of values (l_1, l_2) and M for (m_1, m_2). Then the equation (4) becomes

$$\left\{\frac{d^2}{dR^2}+k_L{}^2-\frac{j(j+1)}{R^2}-2\mu(LMjm|V|LMjm)\right\}g^{jm}_{LM}$$
$$=2\mu\sum{}'(LMjm|V|L'M'j'm')g^{j'm'}_{L'M'}, \tag{4'}$$

where the prime on $\sum$ denotes the omission of the diagonal term. In the approximate method of distorted wave, this set of equations is replaced by

$$\left\{\frac{d^2}{dR^2}+k_0{}^2-\frac{j(j+1)}{R^2}-2\mu(L_0M_0j0|V|L_0M_0j0)\right\}g^{j0}_{L_0M_0}=0 \tag{4'a}$$

$$\left\{\frac{d^2}{dR^2}+k_L{}^2-\frac{j(j+1)}{R^2}-2\mu(LMjm|V|LMjm)\right\}g^{jm}_{LM}$$
$$=2\mu\sum_{j'}(LMjm|V|L_0M_0j'0)g^{j'0}_{L_0M_0}. \qquad (LM\neq L_0M_0) \tag{4'b}$$

Then we take the solution of the equation (4'a) which vanishes at the origin and are normalized by the following asymptotic form*)

*) If the scattering potential is spherically symmetric, the wave function representing the incident and the scattered waves has the following general form:

$$f(\boldsymbol{R})=\sum_{n=0}^{\infty}(2n+1)i^n\exp(i\eta_n)L_n(R)_nP(\cos\Theta),$$

where $L_n(r)$ is the solution of the homogeneous radial equation which becomes asymptotically $(kr)^{-1}\sin(kr-n\pi/2+\eta_n)$. (See reference (6), Chap. II, § 1.)

$$\sqrt{4\pi}\, i^j \exp(i\eta_j)\, \sin(k_0 R - j\pi/2 + \eta_j)/k_0 .$$

Let us call this solution $G^{j0}_{L_0M_0}$ (or G^j_0 for brevity). Such normalization corresponds to the incident plane wave of unit amplitude, i.e., $\exp(ik_0 R\cos\theta)$. Then substituting this initial state wave function $G_0{}^{j0}$ into the right hand side of the equation (4'b) we have the inhomogeneous equation for the final state wave function ($L \neq L_0$). The equation of this form can be solved formally[5,7,8] and its solution has the following asymptotic form

$$g^{jm}_{LM} \sim -(2\mu/\sqrt{4\pi})\exp(ik_L R + i\eta_L) \times \sum_{j'} \int_0^\infty G^{jm}_{LM}(LMjm|V|L_0M_0j'0)\, G^{j'0}_0\, dR \qquad (R\to\infty), \tag{5}$$

where G^{jm}_{LM} is the solution of the homogeneous equation obtained from (4'b), which vanishes at the origin and is normalized asymptotically as

$$\sqrt{4\pi}\, \sin(k_L R + \eta_L)/k_L .$$

It is noted that the summation on j' is contained in the equation (5) which causes the mutual interference between the partial waves with different orbital angular momenta. This effect originates in the fact that the intermolecular force potential is not spherically symmetric.

As is well known, if the wave function f has the asymptotic form

$$f_{LM}(\boldsymbol{R}) \sim \exp(ik_L R) F_{LM}(\Theta, \Phi)/R \qquad (R\to\infty),$$

then the total cross section for the transition $L_0M_0 \to LM$ is defined by

$$Q_{LM} = (k_L/k_0)\int |F_{LM}|^2 d\Omega .$$

Therefore we have from (4a) and (5) that

$$\begin{aligned} Q_{LM} &= (k_L/k_0)\sum_{j,m}(2j+1)\,|g^{jm}_{LM}(R\to\infty)|^2 \\ &= (1/4\pi)(k_L/k_0)\sum_{j,m}(2j+1)\,\Big|\int_0^\infty 2\mu G^{jm}_{LM} \sum_{j'}(LMjm|V|L_0M_0j'0)\, G^{j'0}_0\, dR\Big|^2 . \end{aligned} \tag{6}$$

Finally, the cross section for the process $L_0 \to L$ is given by

$$Q_L = \frac{1}{(2l_{10}+1)(2l_{20}+1)} \sum_{MM_0} Q_{LM}, \tag{6'}$$

and this completes our formulation based on the distorted wave approximation.

§ 3. Matrix elements of the intermolecular force potential for the two diatomic molecules

In this section, we consider the collision of two homonuclear diatomic molecules, i.e., of the type $A_2 + B_2$. The main force which contributes to the inelastic collision cross section is the strong repulsive force acting at small distance of approach. Thus we may safely neglect the van der Waals force. We further assume that the intermolecular force

potential is given by the sum of the interaction potential $\varphi(r)$ for the four pairs of atoms belonging to the different molecules.[9] In the thermal collisions, the closest distance of approach is much larger than the interatomic distances inside the molecules. Then we take only the first two terms of the Taylor expansion which give[3]

$$V=4\varphi(R)+(1/2)(d^2\varphi(R)/dR^2)(\xi_1^2\cos^2\chi_1+\xi_2^2\cos^2\chi_2).$$

The interatomic potential $\varphi(r)$ is usually approximated by a function of the form: $const\times exp(-\alpha r)$. Therefore, it is sufficient for our problem to consider the potential of the form

$$V=\{\beta+(\gamma_1\cos^2\chi_1+\gamma_2\cos^2\chi_2)\}\exp(-\alpha R). \tag{7}$$

In another form we may write

$$V=\{a+b_1P_2(\cos\chi_1)+b_2P_2(\cos\chi_2)\}\exp(-\alpha R), \tag{7'}$$

where $a=\beta+(\gamma_1/3)+(\gamma_2/3)$, $b_i=2\gamma_i/3$.

The matrix elements $(l_1m_1l_2m_2jm|V|l_1'm_1'l_2'm_2'j'm')$ of the potential (7') are calculated easily. By remembering the addition theorem

$$P_n(\cos\chi_i)=(4\pi/2n+1)\sum_{m=-n}^{n}Y_{nm}^*(\theta_i,\varphi_i)\,Y_{nm}(\Theta,\Phi),$$

and using the abbreviation[10]*)

$$C^L(l'm',lm)=(2/2L+1)^{1/2}\delta(m+M,m')\int_0^\pi\Theta_{lm}(\theta)\,\Theta_{LM}(\theta)\,\Theta_{l'm'}(\theta)\sin\theta\,d\theta,$$

we have from (3b) and (4b)

$$\begin{aligned}&(l_1m_1l_2m_2jm|V|l_1'm_1'l_2'm_2'j'm')\\&=(2j'+1/2j+1)^{1/2}\big[a\delta(l_1,l_1')\delta(m_1,m_1')\delta(l_2,l_2')\delta(m_2,m_2')\delta(j,j')\delta(m,m')\\&\quad+b_1C^2(jm,j'm')C^2(l_1'm_1',l_1m_1)\delta(m_1+m,m_1'+m')\delta(l_2,l_2')\delta(m_2,m_2')\\&\quad+b_2C^2(jm,j'm')C^2(l_2'm_2',l_2m_2)\delta(m_2+m,m_2'+m')\delta(l_1,l_1')\delta(m_1,m_1')\big]\exp(-\alpha R).\end{aligned} \tag{8}$$

The selection rule $j-j'=0,\pm2$ is derived from the property of the coefficients $C^2(jm,j'm')$. The diagonal elements are given by

$$\begin{aligned}&(l_1m_1l_2m_2jm|V|l_1m_1l_2m_2jm)\\&\quad=[a+C^2(jm,jm)\{b_1C^2(l_1m_1,l_1m_1)+b_2C^2(l_2m_2,l_2m_2)\}]\exp(-\alpha R).\end{aligned} \tag{8'}$$

The values of $C^2(lm,l'm')$ are listed in the Condon-Shortley's text[10] (p. 178) and Shortley-Fried's paper[11] for the not too large values of l and l'. For the larger values of l and l', one has to calculate these coefficients from the general formulae. (See Appendix II.)

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*) $Y_{lm}(\theta,\varphi)=\Theta_{lm}(\theta)\Phi_m(\varphi)$. Do not confuse the function $\Theta_{lm}(\theta)$ and $\Phi_m(\varphi)$ with the Θ and Φ which are the angular components of the vector $\boldsymbol{R}$.

§ 4. Approximate solution of the homogeneous radial equation

Now we are forced to enter into a difficult problems, i.e., the solution of the radial equations. The general form of them in our approximation is

$$\left\{\frac{d^2}{dR^2}+k^2-\frac{j(j+1)}{R^2}-Ae^{-BR}\right\}\varphi(R)=0. \tag{9}$$

When we require only the elastic scattering cross section, all we have to calculate is the asymptotic behaviour of the wave function (i.e., phase shift). But, we need to know the entire wave function in our problem. Moreover, since, in the molecular collisions, a large number of the partial waves contribute to the cross section even at the thermal energy, we must solve a very large number of the radial equations. Therefore it is desirable to make some simplifications according to the required accuracy. In the following we consider the various methods of solution:

(i) *Numerical integration*

This is the most rigorous method of the calculation if it is done thoroughly. Starting from the initial condition $\varphi(0)=0$ and $(d\varphi/dR)_{R=0}=a\ const.$ at the origin, the entire form of the function φ is obtained successively. (See for example Mott-Massey: reference (6) Chap. VII, § 6.4.) The undetermined factor is fixed by the condition that the solution obtained must be properly normalized for the large separation where

$$k^2 \gg j(j+1)/R^2+A\exp(-BR).$$

(ii) *WKB-approximation*

The well-known method of Wentzel, Kramers and Brillouin may be used for our purpose. In the neighbourhood of the classical turning point, $R=\bar{R}$, where $k^2=j(j+1)/\bar{R}^2-A\exp(-B\bar{R})$, the WKB approximation becomes invalid. In this region we may approximate the potential function as a linear one so that the solution is approximated by a Bessel function of the order 1/3. (See for example Schiff: reference (12), § 28.)

(iii) *Variational method*

This method is employed by Erskine and Massey[13] for the electron impact. Of course this is the method appropriate to determine the phase shift and not suitable to get the wave function itself. Yet, this may be used conveniently because sometimes we require only the rough features of the distorted wave function when the accuracy aimed at is not so high.

(iv) *Method of modified wave number*

Let us consider the gradients of the two terms in the effective potential

$$j(j+1)/R^2+A\exp(-BR). \tag{10}$$

For example if j is not so large the curve representing the first term is very flat compared with the second one at least near the classical turning point. (see fig. 2.) Then the first term may be taken as a constant in this region. In other words, wave number k is replaced by the modified wave number

$$\tilde{k}=\{k^2-j(j+1)/\bar{R}^2\}^{1/2} \quad (11)$$

and our problem reduces to the S-wave problem, which is easy to handle.

(v) *Classical approximation*

Let us assume that the molecules are spherical and that the transition probability depends only upon the relative velocity $v_\parallel$ along the line joining the centers at collision. Such assumption is usually made when one treats the chemical reaction in gas phase by the classical kinetic theory of gases. In our problem, we have the following foundation of this assumption:

(a) The diatomic molecules are dumb-bell-like for the colliding particles with high energy, but they are not so far from spherical for the thermal energy particles.

(b) The motion of the molecule can be treated classically if the velocity is not so small. (Note that the contributions to the transition rate from the collisions with very small relative velocities are usually negligible.)

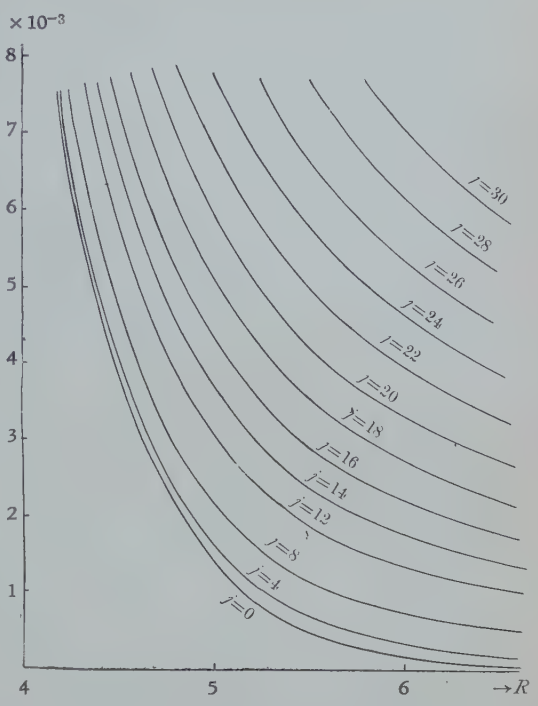

Fig. 2. An example of the effective potential curve: $A\exp(-2R)+j(j+1)/2\mu R^2$ ($A=30.7$, $2\mu=3675.0$).

(c) If the collision diameter (sum of the molecular radii) is $\bar{R}$ and if the relative velocity is v, then the angular momentum is

$$j=\mu v\bar{R}\sin\theta_j\,.$$

(see fig. 3.) On the other hand $v_\parallel=v\cos\theta_j$: Thus we get

$$(\mu v_\parallel)^2=(\mu v)^2-(j/\bar{R})^2, \quad (11')$$

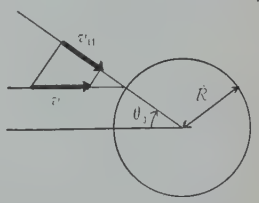

Fig. 3

which is identical with (11) except that j^2 in (11′) is replaced by $j(j+1)$ in (11). Therefore, our assumption is not so unreasonable.

If we admit this assumption, only the transition probability in the head-on collision (or S-wave collision, wavemechanically) is required. Let $P_0(k_i)$ be the transition probability per collision for the S-wave (k_i=initial wave number), then the number of transitions occuring in unit volume of gas phase per unit time is given by

$$\int_0^\infty P_0(\mu v_\parallel)f(v_\parallel)dv_\parallel$$

$$=\int_0^\infty P_0(\mu v_\parallel)2nn'\bar{R}^2(2\pi\mu/kT)^{1/2}\exp(-\mu v_\parallel{}^2/2kT)v_\parallel dv_\parallel\equiv n'\varkappa\,. \quad (12)$$

For the transition of the type: $A^*+B\rightarrow A+B$ (asterisk means the excited state), n' is the number density of molecules A^*, n is that of the collision partner B. $f(v_\parallel)dv_\parallel$ is the number of collisions among A^*- and B-molecules per unit time and per unit volume, in which the relative velocity along the line joining their centers lies in the range $v_\parallel$, $v_\parallel+dv_\parallel$.[14] k is the Boltzmann's constant and T stands for the absolute temperature.

§ 5. Numerical calculation for the H_2-molecule by the classical approximation. Comparison with the experimental evidence

Let us now apply the classical approximation to the rotational transition of H_2-molecule. As an example we consider the following transition:

(initial state) $\cdots l_1=2$; $m_1=\pm 2, \pm 1, 0$; $l_2=m_2=0$; $(m=0)$;

(final state) $\cdots l_1=m_1=0$; $l_2=m_2=0$; (final value of m=initial value of m_1).

In the final state, we have two idetical H_2-molecules. Then the angular momentum of the relative motion is limited to the even number, i.e., $j=0, 2, 4, \cdots$, which is the characteristic feature of the Bose statistics. But the matrix elements of the potential obtained in § 3 show that $j-j'=0$ or ± 2. Therefore the initial state with odd value of j' can not be combined with any final state. Correspondingly we must multiply the transition rate formula (12) by the factor $1/2$.

Following the programme of the classical approximation, we first consider the case in which $j=j'=0$. Then the incident wave and its elastically scattered wave is asymptotically

$$\begin{aligned}&\exp(-ik_iR)/R+A_i\exp(ik_iR)/R \qquad (R\rightarrow\infty)\\ &=2\exp(i\eta)\cos(k_iR+\eta)/R \qquad (A_i=\exp(2i\eta)).\end{aligned}$$

On the other hand, the asymptotic form of the inelastically scattered wave is

$$A_f\exp(ik_fR)/R\,.$$

The transition probability per collision is given by

$$P_0=(k_f/k_i)|A_f|^2.$$

Now the S-wave component of the initial state wave function considered in § 2 is normalized asymptotically as

$$(1/k_iR)\times\text{sinusoidal funtion.}$$

Therefore the contribution Q_0 to the equation (6′) from the term with $j=j'=0$ is related with P_0 by

$$P_0=(1/4\pi)(2k_i)^2Q_0=(k_i^2/\pi)Q_0\,. \tag{13}$$

Q_0 is from (6), (6′)

$$Q_0=(1/5)\sum_m(1/4\pi)(k_f/k_i)|2\mu\textstyle\int_0^\infty G_f^{00}V_0G_i^{00}dR|^2, \tag{14}$$

where V_0 is the matrix element (4b) of the potential V for the transition considered $(j=j'=0)$. However, we know from the previous section that the S-wave is the representa-

tive of the other partial waves in our calculation. It seems better, therefore, to replace the matrix element V_0 by the average of

$$V_j=\sum_{j'}(final,\ j,\ m|\ V|initial,\ j',\ 0).$$

(See the equation (6). We have assumed here that the phase shift $\eta_{jj'}$ does not change rapidly with j'.) We get from the equation (8) and the Appendix II that

$$V_j=\sum_{j'=j,j\pm 2}(2j'+1/2j+1)^{1/2}b_1C^2(jm,j'0)C^2(2m,00)\exp(-aR).$$

Fortunately, V_j converge rather rapidly to a limiting value when j increases. Thus we may adopt $\lim_{j\to\infty} V_j$ as the average. The results of calculation is

$$\bar{V}=\lim_{j\to\infty} V_j=b_1\exp(-aR)\times\begin{cases}0.4472, & (m=0),\\ 0, & (m\neq 0).\end{cases}$$

Putting this $\bar{V}$ into the equation (14) and combining this with the equation (13), we get

$$P_0=0.4408\sinh(\pi k_i)\sinh(\pi k_f)/(\cosh(\pi k_f)-\cosh(\pi k_i))^2, \qquad (15)$$

where we have used Jackson-Mott's formula[15] (see Appendix III) and the following values of constants: $2\mu=3675.0$ atomic units, ΔE (energy difference between the initial and the final rotational states) $=1.65\times 10^{-3}$ atomic units. As to the potential $V(R)$, see Appendix I.

Substituting above P_0 into the equation (12) and multiplying a factor 1/2 representing the effect of statistics mentioned above, we find, for $T=197.7°$K, 1 atmospheric pressure, that

$$\varkappa_{calc}=0.55\times 10^{-10}\bar{R}^2 \text{ atomic units.}$$

This quantity is the transition probability of an excited H_2-molecule in gas phase to the ground state per unit time ($=2.42\times 10^{-17}$ sec). This value can be compared with the experimental value obtained by J. E. Rhodes.[2] From the measurement of the anomalous dispersion of the supersonic wave in the pure para hydrogen gas, he obtained for the "relaxation frequency to pressure ratio"

$$(f/p)_0=(\varkappa/2\pi p)(1+5\exp(-\Delta E/kT))=6.6\pm 0.3\times 10^6 \text{ sec}^{-1}\text{ atm.}^{-1}$$

for $T=197.7°$K. Thus putting $p=1$ atm., we have

$$\varkappa_{obs}=7.4\times 10^{-10} \text{ atomic units.}$$

Equating $\varkappa_{calc}$ and $\varkappa_{obs}$, we obtain $\bar{R}=3.7$. But the integrand of the integral in (12) has its maximum value near $k_i=2.0$ and the corresponding value of the classical turning point distance is $R=5.1$. If we use this value for R, we get $\varkappa_{calc}=14.2\times 10^{-10}$. Of course the collision diameter is not identical with the classical turning point distance and this ambiguity is inevitable in our approximation method. In any case the result of our calculation agrees with the experimental one within a factor 2 and this agreement is much better than is expected because we have used the much simplified method of calculation and we have no decisive knowledge about the intermolecular force potential.

§ 6. Conclusion

Because of the essentially complex feature of the problem, we have made many simplifications. Among others the classical approximation for the solution of the radial equation is considerably rough, though it has an advantage in simplicity. Thus the solution of the radial equation by a more rigorous method (e.g., by WKB-approximation) is desired. On the other hand, it is also desirable to apply the various methods of approximation (including the classical approximation) to other processes. We are planning such calculations.

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Appendix I. Interaction potential between two hydrogen molecules

As stated in § 3, we assume for the form of the interaction potential as follows:

$$V(R,\chi_1,\chi_2)=4\varphi(R)+(\xi^2/2)\varphi''(R)(\cos^2\chi_1+\cos^2\chi_2).$$

Here ξ is the internuclear distance inside the hydrogen molecule, and its value is 1.44 atomic units. For the potential function $\varphi(r)$ between two atoms, we have had no decisive knowledge. J. de Boer[9] obtained approximately that

$$\varphi(r)=2.78\exp(-1.87r) \text{ atomic units.}$$

Using this function, we are led to

$$V(R)=[11.1+10.1(\cos^2\chi_1+\cos^2\chi_2)]\exp(-1.87R).$$

Another detailed calculation of V was performed independently by Margenau.[16] His results are approximately expressed by

$$V(R)=60\exp(-2.22R)+16\exp(-2R)(\cos^2\chi_1+\cos^2\chi_2).$$

In the most important region in our calculation where R is near 5 atomic units, we may use more simple form

$$V(R)=[20+16(\cos^2\chi_1+\cos^2\chi_2)]\exp(-2R).$$

The absolute value of this function V and its dependence on R are not so far from the semi-empirical formula given by Buckingham and Corner.[17] We used this form in § 5.

Appendix II. The coefficients $C^k(lm,l'm')$

Definition and general formula (See reference (10).)

$$C^k(lm,l'm')=(-1)^{m-m'}C^k(l'm',lm)$$
$$\equiv(2/2k+1)^{1/2}\int_0^\pi\Theta(k,m-m')\Theta(l,m)\Theta(l',m')\sin\theta\,d\theta$$
$$=\frac{(-1)^{g-k-m'}(2g-2l')!\,g!}{(g-k)!\,(g-l)!\,(g-l')!\,(2g+1)!}\times$$

$$\left[\frac{(2l+1)(2l'+1)(l-m)!\,(k+m-m')!(l'+m')!(l'-m')}{(l+m)!\,(k-m+m')!}\right]^{1/2}\times$$

$$\sum_t(-1)^t\frac{(l+m+t)!\,(k+l'-m-t)!}{(l-m-t)!\,(k-l'+m+t)!\,(l'-m'-t)!\,t!},$$

provided that $2g=k+l+l'=even$ and $|l-l'|\leqq k\leqq l+l'$. The function $\theta(l,m)$ is defined by

$$\theta(l,m)=(-1)^m\left[\frac{2l+1}{2}\frac{(l-m)!}{(l+m)!}\right]^{1/2}\sin^m\theta\frac{d^m}{(d\cos\theta)^m}P_l(\cos\theta),$$

$$\theta(l,-m)=(-1)^m\theta(l,m). \qquad (m>0)$$

Some formulae with even j.

$$C^2(j,0;j,0)=\frac{j(j+1)}{(2j-1)(2j+3)},$$

$$C^2(j,0;j+2,0)=C^2(j+2,0;j,0)=\frac{3}{2}\frac{(j+1)(j+2)}{(2j+1)(2j+3)}\left(\frac{2j+1}{2j+5}\right)^{1/2},$$

$$C^2(j,1;j,0)=\frac{[6j(j+1)]^{1/2}}{2(2j-1)(2j+3)} \qquad (j\neq 0),$$

$$C^2(j,1;j+2,0)=-\frac{j+2}{2(2j+3)}\left[\frac{6j(j+1)}{(2j+1)(2j+5)}\right]^{1/2} \qquad (j\neq 0),$$

$$C^2(j,1;j-2,0)=\frac{j-1}{2(2j-1)}\left[\frac{6j(j+1)}{(2j-3)(2j+1)}\right]^{1/2} \qquad (j\neq 0),$$

$$C^2(j,2;j,0)=-\frac{[6(j-1)j(j+1)(j+2)]^{1/2}}{2(2j-1)(2j+3)} \qquad (j\neq 0),$$

$$C^2(j,2;j+2,0)=\frac{1}{4(2j+3)}\left[\frac{6(j-1)j(j+1)(j+2)}{(2j+1)(2j+5)}\right]^{1/2} \qquad (j\neq 0),$$

$$C^2(j,2;j-2,0)=\frac{1}{4(2j-1)}\left[\frac{6(j-1)j(j+1)(j+2)}{(2j-3)(2j+1)}\right]^{1/2} \qquad (j\neq 0).$$

Appendix III. Solution of the S-wave equation

In the equation

$$\left\{\frac{d^2}{dR^2}+k^2-A\exp(-BR)\right\}\varphi(R)=0$$

we make the change of variable

$$y=(2\sqrt{A}/B)\exp(-BR/2).$$

Then we get

$$\left\{\frac{d^2}{dy^2}+\frac{1}{y}\frac{d}{dy}+\left(\frac{2k}{B}\right)^2\frac{1}{y^2}-1\right\}\varphi(y)=0.$$

Jackson and Mott[15]'s solution : $\varphi(R)=const.\ K_{iq}(y)$, where $q=2k/B$, is the solution which vanishes at $R\to-\infty\,(y\to+\infty)$. We must take the solution which vanishes at the origin. However, in the slow collisions, the wave function decreases rather rapidly inside the classical turning point and hardly reaches the origin. In this case the solution which we require is almost same with the Jackson-Mott's solution, which is

$$\varphi(R)=2(q\sinh\pi q)^{1/2}K_{iq}(y)/k$$

under the normalization as in § 2.

In the case for which the calculation is performed in § 5, the potentials of the elastic scattering are

$$[a+b_1C^2(j,0\,;j,0)C^2(l_1,m_1\,;l_1,m_1)]\exp(-\alpha R)$$

for the initial state and $a\exp(-\alpha R)$ for the final state. (See the equation (8′).) Here the term containing b_1 is much smaller than a and therefore negligible. Thus we put $A=a$, $B=\alpha$.

The matrix element of $2\mu b_1\exp(-\alpha R)$ held between above φ-functions (initial and final) is obtained directly following the calculation by Jackson and Mott. The resulting formula is

$$2\mu b_1\int_0^\infty\varphi(final)\exp(-\alpha R)\varphi(initial)dR\fallingdotseq 2\mu b_1\int_{-\infty}^{\infty}\cdots$$

$$=\frac{b_1}{a}\frac{\alpha\pi^2}{k_ik_f}\frac{(q_iq_f\sinh\pi q_i\sinh\pi q_f)^{1/2}(q_f^2-q_i^2)}{2(\cos\pi q_f-\cosh\pi q_i)}\qquad\left(q=\frac{2k}{\alpha}\right),$$

from which we get the equation (15).

References

1) K. Takayanagi, Prog. Theor. Phys. **8** (1952), 111.
2) J. E. Rhodes, Phys. Rev. **70** (1946), 932.
3) A. S. Roy and M. E. Rose, Proc. Roy. Soc. **A149** (1935), 511.
4) C. F. Curtiss, J. O. Hirschfelder and F. T. Adler, J. Chem. Phys. **18** (1950), 1638.
5) C. F. Curtiss and F. T. Adler, J. Chem. Phys. **20** (1952), 249.
6) N. F. Mott and H. S. W. Massey, *The theory of atomic collision* (1949).
7) C. Zener, Phys. Rev. **37** (1931), 556.
8) reference (6) p. 108.
9) J. de Boer, Physica **9** (1942), 363.
10) E. U. Condon and G. H. Shortley, *Theory of atomic spectra* (1935).
11) G. H. Shortley and B. Fried, Phys. Rev. **54** (1938), 739.
12) L. I. Schiff, *Quantum mechanics* (1949).
13) G. A. Erskin and H. S. W. Massey, Proc. Roy. Soc. **A212** (1952), 521.
14) See e.g. H. J. Schumacher, *Chemische Gasreakti nen* (1938).
15) J. M. Jackson and N. F. Mott, Proc. Roy. Soc. **A137** (1932), 703.
16) H. Margenau, Phys. Rev. **64** (1943), 131.
17) R. A. Buckingham and J. Corner, Proc. Roy. Soc. **A189** (1947), 118.

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The j–j Coupling Shell Model

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A j–j coupling shell model of nucleus is proposed. The theory of j–j coupling in nuclei is developed. By making use of this extended theory about spin eigenfunctions in j–j coupling, nuclear magnetic moments are calculated, and the results are in agreement with experiments. The data on β-decay are also consistent with the present j–j coupling shell model.

§ 1. Introduction

The difference between the theory of j–j and L–s coupling, which is due to the half-integer values of j, is easily overcome by making use of the symplectic transformation[1].

By utilization of this extended theory about spin eigenfunctions in j–j coupling, we are able to calculate the nuclear magnetic moments and show that nuclear spins and magnetic moments are well explained by the present model, in which several assumptions are introduced.

§ 2. Symmetry of spin functions

The nuclear wave function of a system with n particles in the outermost orbit is written as

$$\Psi = \Psi(\text{inner})\Re(r)\cdot\Pi^{\nu}\psi(j^{\nu})\tau(j^{\nu})$$

$\Psi(\text{inner})$ is the spin function of the nucleons in the closed shell. $\Re(r)$ is the radial wave function in the sense of j–j coupling, and $\tau(j^{\nu})$ is the isotopic spin function.

As is well known, the symmetry character of the isotopic spin part is the same as that of the spin (not the total spin) part in the sense of the atomic spectra. The symmetry character of the space spin part $\psi(j)$ in the sense of j–j coupling is obtained by the decomposition of the character of the regular representation[2].

In the case of $j \leq 5/2$ it is necessary to introduce for the spin eigenfunction a primitive structure which is peculiar to nuclei and a seniority number, which is the analogue of the seniority number in atomic spectra[3].

The nuclear eigenfunction is represented as the linear combination of some linearly independent bases. The linearly independent bases are separated into several groups by the number of pairs which are coupled to give an invariant antisymmetric bilinear form of zero angular momentum and to give unit isotopic spin

$$\sum_{m}(-1)^{m-1/2}\phi_{m}(i)\phi_{-m}(k)\tau_{\xi}^{1}(i,k),$$

The character of the spin function with each seniority number is obtained inductively by subtracting the character of the spin function with seniority number $s_j=n-2,\ n-4,$ ……from the character of the spin function of the n-particle system.*

Here the following fact is to be noted. We are also able to consider the seniority number s_τ due to the isotopic spin eigenfunction if a charge invariant nuclear interaction is assumed, but since the individual isotopic spin τ is a dichotomic variable, the irreducible representation of the permutation group has also the definite seniority number s_τ.

Then the spin eigenfunction of the n-particle system, whose seniority number is s_j, is represented as the linear combination of some independent bases, that is

$$\sum_P \epsilon_P P \sum_{\xi,\xi',t_\xi,t} k^t_{\xi',\xi,t_\xi} \psi^0(1,2)\cdots\psi^0(n-s_j-2,\ n-s_j-1)\psi^{r'}(s_j) \times \tau^1_\xi(1,2)\cdots\tau^1_{\xi'}(n-s_j-2,\ n-s_j-1)\tau^t_{t_\xi}(s_j)$$

where $\psi^0(1,2)$ is the rotationally invariant antisymmetric bilinear form, and P is the permutation operator, and $\epsilon_P=\pm1$ for P odd or even respectively.

Since we assume that the interaction between nucleons is charge invariant, this spin eigenfunction of the n-particle system with seniority number s_j, breaks up in the following way :

$$\sum_P \epsilon_P P \sum_{\xi,\xi',t_\xi} k^t_{\xi,\xi',t_\xi} \psi^0(1,2)\cdots\psi^0(n-s_j-2,\ n-s_j-1)\psi^{r'}(s_j) \times \tau^1_\xi(1,2)\cdots\tau^1_{\xi'}(n-s_j-2,\ n-s_j-1)\tau^t_{t_\xi}(s_j)$$

which has the definite residual isotopic spin t. We call $(s_j,\ t)$ " the primitive structure." In the following we denote simply the primitive structure by $(s,\ t)$ instead of $(s_j,\ t)$.

§ 3. Explicit form of the spin eigenfunction

In order to calculate the nuclear magnetic moment, it is necessary for us to construct the nuclear spin eigenfunction explicitly.

We now introduce the " symplectic representation " in which we make the unit matrix represent the permutation operator which acts on the antisymmetric bilinear form

$$\sum_m (-1)^{m-1/2}\phi_m(i)\phi_{-m}(k).$$

Then the representations of the symplectic transformation and ordinary transformation replace one another.

We denote the partition[5] in the symplectic representation by $[\lambda]_{sp}$, it is clear that

$$[\lambda]_{sp}=[\lambda]^t.$$

In the following we will use the symplectic representation for the representation of the space spin eigenfunction in the sense of j–j coupling and the ordinary representation

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* This procedure is easy and convenient for the classification of the nuclear states of special nuclei only. For the complete table of the classification of nuclear states, see Flowers' excellent work[4].

for the representation of isotopic spin eigenfunction. Then the total eigenfunction is written as

$$\Psi = \psi([\lambda]_{sp}) \cdot \tau([\lambda]).$$

The above considerations suggest that the total eigenfunction of the partition $[\lambda_1, \lambda_2]$ in isotopic spin space (that is, $T=(|\lambda_1-\lambda_2|/2)$) should be represented as

$$\sum_P \epsilon_P P \sum k^{J_1,J_2}_{m,m'} \overbrace{\psi_m(\lambda_1)}^{J_1} \overbrace{\psi_{m'}(\lambda_2)}^{J_2} \cdot \sum k_{\zeta,\zeta'} \overbrace{\tau_\zeta(\lambda_1)} \overbrace{\tau_{\zeta'}(\lambda_2)}.$$

$\overbrace{\psi(\lambda)}$ is the totally antisymmetric function and $\overbrace{\tau(\lambda)}$ is the totally symmetric eigenfunction, and its partition is $[\lambda]$. $\sum k_{mm'} \overbrace{\psi_m(\lambda_1)\psi_{m'}(\lambda_2)}$ is the eigenfunction of definite total spin J. $\sum k_{\zeta\zeta'} \overbrace{\tau_\zeta(\lambda_1)\tau_{\zeta'}(\lambda_2)}$ is the eigenfunction of definite total isotopic spin T. The proof is shown in the appendix 1.

Consider the case of λ_1=even, λ_2=odd. If we take $\psi(\lambda_1)$ as an eigenfunction with zero seniority number and zero resultant angular momentum and $\psi(\lambda_2)$ as an eigenfunction with seniority number λ_2 and then of the partition $[\lambda_2]_{sp}$ and the eigenfunction of the resultant angular momentum J, it is clear that this eigenfunction has a primitive structure $(s.t)=(\lambda_2, \lambda_2/2)$.

In heavy nuclei the outermost orbits of neutrons and protons are different, and the neutron orbit corresponding to the outermost proton orbit is already closed. In this case any total eigenfunction has definite total isotopic spin $T=T_\zeta$, and the explicit form of the corresponding eigenfunction is written as

$$\sum_P \epsilon_P P \, k^{J_1,J_2}_{m,m'} \overbrace{\psi_m(\lambda_1)}^{J_1} \overbrace{\psi_{m'}(\lambda_2)}^{J_2} \cdot \underbrace{\overbrace{\tau(\lambda_1)}^{\lambda_1/2}}_{\lambda_1/2} \underbrace{\overbrace{\tau(\lambda_2)}^{\lambda_2/2}}_{-\lambda_2/2}.$$

When λ_1=even aud λ_2=odd and if we take $\psi(\lambda_1)$ as an eigenfunction with zero resultant angular momentum, the magnetic moment of the nucleus is determined only by the second kind of nucleon.

§ 4. Calculation of the nuclear magnetic moment

By making use of the nuclear wave function given above, the magnetic moment can easily be obtained by calculating the average of

$$M_z = \sum_i \{g_{pj}(\tau_{\zeta i}-1) + g_{nj}(\tau_{\zeta i}+1)\} j_{zi}/2.$$

Since the terms of the explicit eigenfunction given above are not independent of one another, we must rewrite the nuclear eigenfunction as a sum of terms which are independent of one another. The results are shown in the appendix 2.

It is impossible to check these results by making use of the normalization condition. Instead, the following equation is useful for checking the results:

$$|\sum_i (\tau_{x_i} \mp \tau_{y_i})\Psi|^2 = (T \mp T_\zeta)(T \pm T_\zeta + 1),$$

§ 5. The nuclear shell model

—— nuclei with less than 28 neutrons or protons ——

As will be shown in the detailed discussion of section VIII, the following assumptions are adequate to explain the nuclear magnetic moments and spins in all cases without exception :

(1) The succession of energies of nucleon orbits is : $1s$, $2p_{3/2}$, $3p_{1/2}$, $3d_{5/2}$, $2s_{1/2}$, $3d_{3/2}$, $4f_{7/2}$.

It is not necessary to consider that the $d_{5/2}$ and $s_{1/2}$ levels are sometimes crossed and have approximately the same energy as considered by Mayer[6].

(2) The total nuclear wave function is represented by a totally antisymmetric wave function.

As is well known, a system of one kind of nucleons must satisfy the Pauli principle, and the Pauli principle between neutrons and protons has not been absolutely needed. But since, on account of the meson interaction, one nucleon has two states—proton and neutron—it is reasonable and necessary to apply the Pauli principle between nucleons instead of neutrons and protons separately.

(3) The interaction between nucleons is charge invariant and thus total isotopic spin T is conserved.

This is for example the case in neutral meson theory and symmetrical meson theory. The charged meson theory is excluded.

(4) The ground state of the nucleus has minimum total isotopic spin ($T=T_z$).

The energy level spacing in a total isotopic spin multiplet is larger that that in a spin multiplet and that due to different primitive structures.

In addition to the above assumptions, the following subsidiary assumption is adequate with the exception of two special cases.

(5) The ground state of odd A nuclei with λ_1 neutrons and λ_2 protons has primitive structure $(s, t)=(\lambda_{odd}, \lambda_{odd}/2)$, where λ_{odd} is $\lambda_1(\lambda_2)$ if $\lambda_1(\lambda_2)$ is odd.

The ground state of odd-odd nuclei has primitive structures $(s, t)=(\lambda_1+\lambda_2, |\lambda_1-\lambda_2|/2)$.

The ground state of even-even nuclei has primitive structure $(0.\ 0)$.

Since the level spacing between the levels of the same total isotopic spin and of different primitive structures or different resultant spin is assumed to be comparatively small, this rule does not always hold, and sometimes another primitive structure give the lowest energy level. Such a situation occurs in F^{19} and V^{51}.

We have no suitable experimental foundation for assigning the primitive structure of even-even nuclei. Only the seniority selection rules in isomeric transitions and β-decay are useful for investigating the primitive structure of even-even nuclei.

According to these assumptions, the spin of the ground state is not determined uniquely, although the possible spin values are restricted. Thus the configuration $(j)^n$ does not always have the state with resultant space spin $J=j$. For example in the configuration $(d_{5/2})^5$, $T=T_z=1/2$, has the resultant spin $3/2$ and $9/2$ but does not have spin $5/2$ if its primitive structure is $(s, t)=(3, 3/2)$ according to the subsidiary assumption given above.

The j–j coupling shell model given above is clearly distinguished from Mayer's one particle shell model[6]* at this point. As will be shown in the detailed discussion, all the spin descrepancies of Mayer's shell model can be explained by the above considerations in the present j–j coupling shell model.

F^{19} and V^{51} are the only two cases for which the subsidiary assumption does not give agreement with experiments; but as will be shown in the detailed discussion, the magnetic moments and spins of F^{19} and V^{51} are well explained by using some other primitive structures.

§ 6. Magnetic moments of odd A nuclei with the equivalent orbit of proton and neutron

In this case the explicit form of the nuclear wave function is written as follows, if λ_1 is odd and λ_2 is even:

$$\sum_P \epsilon_P P \overbrace{\psi(\lambda_1)}^{J} \overbrace{\psi(\lambda_2)}^{0} \sum k_{\zeta\zeta'} \overbrace{\tau_\zeta(\lambda_1)}^{\lambda_1/2} \overbrace{\tau_{\zeta'}(\lambda_2)}^{\lambda_2/2}$$

according to the assumptions stated above.

The contribution of the term $\overbrace{\psi(\lambda_1)}^{J} \overbrace{\psi(\lambda_2)}^{0} k_{\lambda_1/2,-\lambda_2/2} \overbrace{\underset{\lambda_1/2}{\tau(\lambda_1)}}^{\lambda_1/2} \overbrace{\underset{-\lambda_2/2}{\tau(\lambda_2)}}^{\lambda_2/2}$ is much larger than that of the remaining terms and gives a good approximation for the calculation of nuclear magnetic moments. We call this the first approximation.

The first approximation of the nuclear magnetic moment is written as

$$\mu = J \cdot g_{1j}$$

where g_{1j} is the Landé g-factor of the 1st kind of nucleon. Then, according to the present j–j coupling shell model, the following results are seen to hold in general.

The magnetic moments of odd-A nuclei are in the vicinity of the lines connecting the origin and Schmidt's points. Then the magnetic moments of nuclei are on the Schmidt lines or fall between them near a Schmidt line. This fact gives rise to the expectation that nuclear magnetic moments are explainable in a general terms by a shell model. At the same time it is expected that the present shell model will be able to explain the deviations of nuclear magnetic moments from the Schmidt lines. When $J \leq j$, the deviation of the nuclear magnetic moments is clear from the consideration of the above equation. Besides this, as will be shown in the accurate calculations, numerical results for the magnetic moments are written as

$$\mu = g \cdot J \quad \text{where} \quad g = \alpha g_{1j} + \beta g_{2j}$$
$$(\alpha, \beta \geq 0, \text{ and } \alpha \geq \beta.)$$

From this result it is also possible to explain the deviation of nuclear magnetic moments from the Schmidt lines even when $J = j_1$.

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* Recently Flowers proposed another assumption independently. The present assumptions are also clearly distinguished from Flowers' assumption at this point[7].

§ 7. Odd-odd nuclei

Since $S=\lambda_1+\lambda_2$ according to the assumptions given above, zero spin of the ground state of odd-odd nuclei is excluded on general grounds. But if $s\neq\lambda_1+\lambda_2$, zero spin of the ground state is possible. This fact favours the present subsidiary assumption of odd-odd nuclei.

Moreover, according to our assumptions, the spin of a self-conjugate nucleus which has two nucleons in its outermost orbit is restricted to being odd, in agreement with the experimental fact that all the self-conjugate nuclei of this type have odd spins.

According to the above assumptions, in the case of self-conjugate nuclei, the magnetic moment is given as

$$\mu=g\cdot J, \qquad g=(g_{1j}+g_{2j})/2.$$

This preserves Mizushima and the author's previous results and coincides with Feenberg's results.

It is worthwhile to note the following. According to the subsidiary assumptions, seniority selection rules are expected in β-decay and γ-decay, if $s_i-s_f \quad 4$, where s_i and s_f are the seniority numbers of initial and final nucleus respectively.

§ 8. Detailed discussion of spins and magnetic moments

The results of the calculations of nuclear magnetic moments are shown in table 3.

${}_3Li^6$: $(p_{3/2})^2$, $J=1$; ${}_5B^{10}$: $(p_{3/2})^{-2}$, $J=3$. Both self-conjugate nuclei have odd spin states and the above assumptions corroborate the experiments. Instead, the states with $T=$ odd have only even spin and contradict the experiments.

${}_2Li^7$, ${}_4Be^9$: $(p_{3/2})^{\pm 3}$, $J=3/2$. Mizushima and the authors's previous success[8] is preserved in the present shell model.

${}_9F^{19}$: $(d_{5/2})^3$, $J=1/2$. This is the exception to the subsidiary assumption. The primitive structure $(1, \frac{1}{2})$ specified by the subsidiary assumption has the only one state with spin $5/2$ and does not have a state with spin $1/2$. Instead, the alternative structure $(3, \frac{1}{2})$ is able to explain the magnetic moment and spin very well.

In Mayer's shell model the 9th proton has an $s_{1/2}$ orbit, but this model is not adequate to explain the comparative half lives of the O^{19} and Ne^{19} β-decays, as will be shown below.

${}_{10}Ne^{21}$, ${}_{11}Na^{23}$: $(d_{5/2})^{\pm 5}$, $J=3/2$. According to our assumptions the spin $5/2$ is excluded and, instead, the spin $3/2$ and $9/2$ are possible where the magnetic moment and spin expected from the former agrees with experiments.

${}_{12}Mg^{25}$: $(d_{5/2})^3$, $J=5/2$. The magnetic moment of the state with $T=T_z=\frac{1}{2}$ and the primitive structure $(1, \frac{1}{2})$ specified by the subsidiary assumption agrees with experiment, while the magnetic moment of the state with $T=T_z=\frac{1}{2}$ and the primitive structure $(1, \frac{1}{2})$ disagrees with experiment. The results are shown in table 5.

${}_{17}Cl^{35}$: $(d_{5/2})^3$, $J=3/2$. As seen from the table 6, the agreement with experiment is slightly better for $T=3/2$ than for $T=1/2$. But, as the difference between the magnetic

moment of $T=1/2$ and the experimental value is not very large, it seems that the agreement for the magnetic moment with $T=3/2$ is probably accidental, and the ground state of Cl^{35} must be the state with $T=T_\zeta=\frac{1}{2}$ which is specified by the above assumption.

Sc^{45} : $(f_{7/2})^5$, $T=3/2$, $J=7/2$. The magnetic moment expected from the subsidiary assumption agrees with experiment.

${}_{23}V_{28}^{75}$: $(f_{5/2})^{-5}$, $J=7/2$,. This is the other exception to the subsidiary assumption. According to the subsidiary assumption the spin $7/2$ is excluded. Instead, the alternative primitive structure $(1, \frac{1}{2})$ with $T=T_\zeta=3/2$ is able to explain the magnetic moment and spin.

Mn^{55} : $(f_{7/2})^{-3}(f_{5/2})^2$, $J=5/2$. According to the above assumption, the spin $7/2$ is excluded and, instead, the spin $5/2$ is included ; and the magnetic moment of the state with spin $5/2$ agrees with experiment.

§ 9. Alternative interpretation

In the above shell model the magnetic moment of P^{31} is not satisfactorily explained. This defect is avoidable by making use of the following two alternative models in which the assumptions 2, 3, 4 and 5, are preserved, but the assumption 1 is altered by the following assumptions 1′ or 1″.

Alternative assumptions :

The succession of energies of individual nucleon orbits is

1′ $1s_{1/2}$, $2p_{3/2}$, $2p_{1/2}$, $3d_{5/2}$, $3d_{3/2}$, $2s_{1/2}$, $4f_{7/2}$.

1″ $1s_{1/2}$, $2p_{3/2}$, $2p_{1/2}$, $3d_{5/2}$, $3d_{3/2}$, $2s_{1/2}$, $4f_{7/2}$, for neutron orbits,

$1s_{1/2}$, $2p_{3/2}$, $2p_{1/2}$, $3d_{5/2}$, $2s_{1/2}$, $3d_{3/2}$, $4f_{7/2}$, for proton orbits.

The magnetic moments calculated according to these assumptions are given in table 7 and 8.

The assumption 1′ is not adequate since the spin of K^{39} and K^{41} and the magnetic moment of K^{40} is contradicted by experiment.

The assumption 1″ explains the magnetic moment fairly well in all cases. This seems to be a very promising model.

§ 10. Excited states of even-even nuclei

In the present *j–j* coupling shell model, it is quite natural that the first excited state and some of the second excited states of even-even nuclei with unclosed orbits have spin 2 and spin 4 respectively.[8),10)] This experimental law is easily explained by the assumption that the first excited state of even-even nuclei with unclosed orbits should have the primitive structure $(s, t)=(2,1)$ with $T=T_\zeta$, since the primitive structure $(2,1)$ has only even spin.

§ 11. Beta-decay

As indicated in table 9, 10, 11 and 12, the present *j–j* coupling shell model is adequate to explain the β-decay in all but the two cases of C^{14} and O^{14}.

According to the present *j–j* coupling shell model the following selection rules are expected ;

1. *Principal selection rule*

J-forbidden transition

2. *Subsidiary selection rules*
   a. l-forbidden transition
   b. j-seniority forbidden transition
   c. τ-seniority forbidden transition

The l-forbidden transition means that the total spin change and parity change are allowed but the angular momenta l's of the initial and final nucleon orbits are different; for example $d_{3/2}$——$s_{1/2}$[11].

Besides this, if the seniority numbers of the initial and final nuclei differ by more than four, that is $\Delta s \geq 4$, the transition is expected to be inhibited.

In table 13, the large comparative half life of P^{32} may be well explained by an l-forbidden transition.

In table 14, it is interesting to note that the comparative half-lives of the decay of Sc^{44} and Sc^{45} which are seniority forbidden are to some degree larger than those of the other allowed transitions with few exceptions.

In Mayer's shell model, O^{19}——F^{19} is expected to be 2nd forbidden contradicting the experiments[12]. In the present model O^{19} : $(d_{5/2})^3$ $T=T_z=3/2$ is expected to have spin 3/2 instead of 5/2, and F^{19} has spin 1/2, then the allowed transition of O^{19}——F^{19} is well explained.

In the assumption 1″, Mg^{27}, P^{29} and S^{31} are expected to be j-, l-, and l-forbidden respectively contradicting the experiments.

§ 12. Discussion

Although 1″ is able to explain the magnetic moments of nuclei very well, the explanation of β-decay by the assumption 1″ is less satisfactory than the explanation by the original assumption 1. Thus it seems that the experimental facts are in favour of the original j-j coupling shell model and exclude the alternative assumptions.

The deviation of calculated magnetic moments from the experimental ones are appreciable when the nuclei have comparatively large atomic numbers or $T_z \geq 3/2$. The calculated magnetic moments of H^3, Li^7 and Be^9 deviate to the outside of the two Schmidt lines. Beside these nuclei, the calculated magnetic moments deviate forward the inside of Schmidt's lines. These deviations may be attributed to the following, 1) Coulomb interaction between nucleons, which does not hold the total isotopic spin at $\boldsymbol{T}=\sum_i \tau_i$; 2) exchange moments; 3) angular momentum quantum number li of the individual nucleon is only approximately a good quantum number; 4) the total angular momentum quantum number j_i of the individual nucleon is only approximately a good quantum number.

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It is my pleasant duty to express my hearty gratitude to Professors M. Kotani, S. Nakamura and Y. Yamanouchi for their helpful criticism and encouragement and also to Professor M. Sasaki and Dr. M. Taketani for their kind discussions.

Appendix 1

For example, consider the case of $T=1/2$ and $\nu=5$. The regular representation R, whose bases are

$$\begin{pmatrix}
\alpha(1)\alpha(2)\beta(3)\beta(4)\beta(5)\\
\alpha(2)\alpha(3)\beta(4)\beta(5)\beta(1)\\
\alpha(3)\alpha(4)\beta(5)\beta(1)\beta(2)\\
\alpha(4)\alpha(5)\beta(1)\beta(2)\beta(3)\\
\alpha(5)\alpha(1)\beta(2)\beta(3)\beta(4)\\
\alpha(1)\alpha(3)\beta(2)\beta(4)\beta(5)\\
\alpha(2)\alpha(4)\beta(3)\beta(5)\beta(1)\\
\alpha(3)\alpha(5)\beta(4)\beta(1)\beta(2)\\
\alpha(4)\alpha(1)\beta(5)\beta(2)\beta(3)\\
\alpha(5)\alpha(2)\beta(1)\beta(3)\beta(4)
\end{pmatrix}$$

includes the three irreducible representations, that is;

$$[1^5],\ [21^3],\ [2^21].$$

Thus if ARA^{-1} is the irreducible representation and if $k_{\zeta\zeta'}$'s are chosen so that $\sum k_{\zeta\zeta'}\tau_\zeta\tau_{\zeta'}$ has the resultant isotopic spin $T=1/2$,

$$A\begin{pmatrix}
k_{\zeta\zeta'}\,\tau_\zeta(12)\,\tau_{\zeta'}(345)\\
k_{\zeta\zeta'}\,\tau_\zeta(23)\,\tau_{\zeta'}(451)\\
\cdots\cdots\cdots\cdots\\
\cdots\cdots\cdots\cdots\\
\cdots\cdots\cdots\cdots\\
k_{\zeta\zeta'}\,\tau_\zeta(13)\,\tau_{\zeta'}(245)\\
\cdots\cdots\cdots\cdots\\
\cdots\cdots\cdots\cdots\\
\cdots\cdots\cdots\cdots\\
\cdots\cdots\cdots\cdots
\end{pmatrix}=\begin{pmatrix}
\eta_1\\ \eta_2\\ \eta_3\\ \eta_4\\ \eta_5\\ 0\\ 0\\ 0\\ 0\\ 0
\end{pmatrix}$$

where η_i's are the five bases of the irreducible representation $[2^21]$.

Thus

$$\sum\epsilon_P P\sum k_{mm'}\overbrace{\phi_m(12)\,\phi_{m'}(345)}\cdot\sum k_{\zeta\zeta'}\overbrace{\tau_\zeta(12)}^{\lambda_1/2}\overbrace{\tau(345)}^{\lambda_2/2}$$

$$=\begin{pmatrix}
\sum k_{mm'}\overbrace{\phi_m(12)\,\phi_{m'}(345)}\\
\sum k_{mm'}\overbrace{\phi_m(23)\,\phi_{m'}(451)}\\
\cdots\cdots\cdots\cdots\\
\cdots\cdots\cdots\cdots\\
\cdots\cdots\cdots\cdots\\
-\sum k_{mm'}\overbrace{\phi_m(13)\,\phi_{m'}(245)}\\
-\sum k_{mm'}\overbrace{\phi_m(24)\,\phi_{m'}(351)}\\
\cdots\cdots\cdots\cdots\\
\cdots\cdots\cdots\cdots\\
\cdots\cdots\cdots\cdots
\end{pmatrix}\cdot\begin{pmatrix}
\sum k_{\zeta\zeta'}\overbrace{\tau_\zeta(12)}^{1}\overbrace{\tau_{\zeta'}(345)}^{3/2}\\
\sum k_{\zeta\zeta'}\overbrace{\tau_\zeta(23)}^{1}\overbrace{\tau_{\zeta'}(451)}^{3/2}\\
\cdots\cdots\cdots\cdots\\
\cdots\cdots\cdots\cdots\\
\cdots\cdots\cdots\cdots\\
\sum k_{\zeta\zeta'}\overbrace{\tau_\zeta(13)}^{1}\overbrace{\tau_{\zeta'}(245)}^{3/2}\\
\sum k_{\zeta\zeta'}\overbrace{\tau_\zeta(24)}^{1}\overbrace{\tau_{\zeta'}(351)}^{3/2}\\
\cdots\cdots\cdots\cdots\\
\cdots\cdots\cdots\cdots\\
\cdots\cdots\cdots\cdots
\end{pmatrix}$$

$$= \begin{pmatrix} \sum k_{mm'} \overbrace{\psi_m(12)}\, \overbrace{\psi_{m'}(345)} \\ \cdots\cdots\cdots\cdots \\ \cdots\cdots\cdots\cdots \\ \cdots\cdots\cdots\cdots \\ \cdots\cdots\cdots\cdots \\ -\sum k_{mm'} \overbrace{\psi_m(13)}\, \overbrace{\psi_{m'}(245)} \\ \cdots\cdots\cdots\cdots \\ \cdots\cdots\cdots\cdots \\ \cdots\cdots\cdots\cdots \\ \cdots\cdots\cdots\cdots \end{pmatrix} A^{-1} \cdot A \begin{pmatrix} \sum k_{\zeta\zeta'} \overbrace{\tau_\zeta^{1}(12)}\, \overbrace{\tau_{\zeta'}^{3/2}(345)} \\ \cdots\cdots\cdots\cdots \\ \cdots\cdots\cdots\cdots \\ \cdots\cdots\cdots\cdots \\ \cdots\cdots\cdots\cdots \\ \sum k_{\zeta\zeta'} \overbrace{\tau_\zeta^{1}(13)}\, \overbrace{\tau_{\zeta'}^{3/2}(245)} \\ \cdots\cdots\cdots\cdots \\ \cdots\cdots\cdots\cdots \\ \cdots\cdots\cdots\cdots \\ \cdots\cdots\cdots\cdots \end{pmatrix}$$

$$= \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \\ \phi'_1 \\ \phi'_2 \\ \phi'_3 \\ \phi'_4 \\ \phi'_5 \end{pmatrix} \cdot \begin{pmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \\ \eta_4 \\ \eta_5 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \phi \cdot \eta$$

where ϕ_i's and η_i's are the bases of the irreducible representation $[2^2 1]$.

It is clear from the above consideration that the converse is also true.

Appendix 2

The nuclear spin function which is a representation of both rotational and permutation groups can be constructed as follows:

We start from an invariant formula

$$I = \Pi_{ik} (u_1^{(i)} u_2^{(k)} - u_2^{(i)} u_1^{(k)})^{\sigma_{ik}} \times \Pi_l (u_1^{(l)} x_1 + u_2^{(l)} x_2)^{2j_l - g_l},$$

where $i, k, l = 1, 2, \cdots\cdots, \nu$,

$$g_l = (\sum_k \sigma_{lk} + \sum_k \sigma_{kl}),$$

$$\sum_l 2j_l - \sum g_l = 2J,$$

$$\sum_{i>k} \sigma_{ik} = 2 \sum j_l - 2J.$$

The required eigenfunction $\overbrace{\psi(\lambda)}$ is obtained by antisymmetrizing suitable spin functions given above.

The final result is obtained by representing the nuclear eigenfunction

$$\Psi = \sum \epsilon_P P \sum k_{mm'} \overbrace{\psi_m(\lambda_1)}\, \overbrace{\psi_{m'}(\lambda_2)} \cdot \sum k_{\zeta\zeta'} \overbrace{\tau_\zeta^{\lambda_1/2}(\lambda_1)}\, \overbrace{\tau_{\zeta'}^{\lambda_1/2}(\lambda_2)}$$

as a linear combination of suitable independent bases. Some of the explicit nuclear eigenfunction thus obtained are as follows:

for $\nu = 5$, $j_l = 5/2$, $J = 3/2$, $(s, t) = (3, 3/2)$,

$$\Psi = \frac{1}{N}\sum_P \epsilon_P P\Psi',$$

$$\begin{aligned}\Psi' = {} & 6(\alpha\alpha\alpha)(\beta\beta)\cdot\overbrace{(u_{5/2}u_{-5/2}u_{3/2})}\,\overbrace{(u_{5/2}u_{-5/2})} - 4(\alpha\alpha\alpha)(\beta\beta)\overbrace{(u_{5/2}u_{3/2}u_{-5/2})}\,\overbrace{(u_{3/2}u_{-3/2})} \\ & + 4(\alpha\alpha\alpha)(\beta\beta)\overbrace{(u_{5/2}u_{3/2}u_{-5/2})}\,\overbrace{(u_{1/2}u_{-1/2})} + 4(\alpha\alpha\alpha)(\beta\beta)\cdot\overbrace{(u_{1/2}u_{3/2}u_{-1/2})}\,\overbrace{(u_{5/2}u_{-5/2})} \\ & - 4(\alpha\alpha\alpha)(\beta\beta)\overbrace{(u_{1/2}u_{3/2}u_{-1/2})}\,\overbrace{(u_{3/2}u_{-3/2})} + 5(\alpha\alpha\alpha)(\beta\beta)\overbrace{(u_{1/2}u_{3/2}u_{-1/2})}\,\overbrace{(u_{1/2}u_{-1/2})} \\ & - 2\widetilde{(\alpha\beta,\alpha)}\,\widetilde{(\alpha\beta)}\,\overbrace{(u_{1/2}u_{-1/2},u_{3/2})}\,\overbrace{(u_{5/2}u_{-5/2})} \\ & - 2\widetilde{(\alpha\beta,\beta)}\,(\alpha\alpha)\,\overbrace{(u_{5/2}u_{-5/2},u_{3/2})}\,\overbrace{(u_{3/2}u_{-3/2})} + 2\widetilde{(\alpha\beta\beta)}\,\alpha\alpha\,\overbrace{(u_{1/2}u_{-1/2},u_{3/2})}\,\overbrace{(u_{3/2}u_{-3/2})}\end{aligned}$$

where $\widetilde{(\alpha\beta,\beta)}\,\overbrace{(u_{5/2}u_{-5/2},u_{3/2})} = \{\alpha(1)\beta(2)$

$$+\alpha(2)\beta(1)\}\beta(3)\{u_{5/2}(1)u_{-5/2}(2) - u_{5/2}(2)u_{-5/2}(1)\}u_{3/2}$$

+cyclic change.

The other functions needed in the present calculation can be obtained in the same manner.

References

1) H. Weyl, *The classical groups* (1946), Prin. Univ. Press.
2) T. Inui and T. Yanagawa, *The application of group representations to atoms and molecules* (in Japanese), (1950), Shokabo Press.
3) G. Racah, Phys. Rev. **63** (1943), 367.
   H. A. Jahn and van Wieringen, Proc. Roy. Soc. A (1952), in press.
4) B. H. Flowers, Proc. Roy. Soc. **A210** (1952), 497.
5) D. E. Littlewood, *Theory of group characters* (1950), O.U.P.
6) M. G. Mayer, Phys. Rev. **78** (1950), 16.
7) B. H. Flowers, Phys. Rev. **86** (1952), 254.
8) M. Mizushima and M. Umezawa, Phys. Rev. **85** (1952), 37.
9) E. Feenberg, Phys. Rev. **76** (1949), 1275.
10) Horie, Umezawa, Yamaguchi and Yoshida, Prog. Theor. Phys. **6** (1951), 254.
    M. Goldhaber and A. W. Sunyer, Phys. Rev. **83** (1952), 906.
11) S. Nakamura, Phys. Rev. (1952), (being published).
12) Umezawa, Nakamura, Yamaguchi and Taketani, Prog. Theor. Phys. **6** (1951), 406.

Table 1. Symmetry of wave function

Configuration	T'	Primitive Structure
$(3/2)^3$	1/2	(1, 1/2), (3, 1/2)
	3/2	(1, 1/2)
$(5/2)^3$	1/2	(1, 1/2), (3, 1/2)
	3/2	(1, 1/2), (3, 3/2)
$(5/2)^5$	1/2	(1, 1/2), (3, 1/2), (3, 3/2), (5, 1/2)
	3/2	(1, 1/2), (3, 1/2), (3, 3/2)
	5/2	(1, 1/2)
$(7/2)^3$	1/2	(1, 1/2), (3, 1/2)
	3/2	(1, 1/2), (3, 3/2)
$(7/2)^5$	1/2	(1, 1/2), (3, 1/2), (3, 3/2), (5, 1/2)
	3/2	(1, 1/2), (3, 1/2), (3, 3/2), (5, 3/2)
	5/2	(1, 1/2), (3, 3/2)

Table 2. Primitive structure and spin

Orbit	Primitive Structure	Spin
3/2	(1, 1/2)	3/2
	(3, 1/2)	1/2, 5/2, 7/2
	(3, 3/2)	3/2
5/2	(1, 1/2)	5/2
	(3, 1/2)	1/2, 3/2, 5/2, $7/2^2$, 9/2, 11/2, 13/2
	(3, 3/2)	3/2, 9/2
	(5, 1/2)	1/2, 3/2, $5/2^2$, $7/2^2$, $9/2^2$, $11/2^2$, 13/2, 15/2, 17/2
7/2	(1, 1/2)	7/2
	(3, 1/2)	1/2, 3/2, $5/2^2$, $7/2^2$, $9/2^2$, $11/2^2$, $13/2^2$, $15/2$, 17/2, 19/2
	(3, 3/2)	3/2, 5/2, 9/2, 11/2, 15/2
	(5, 1/2)	$1/2^2$, $3/2^4$, $5/2^5$, $7/2^7$, $9/2^7$, $11/2^7$, $13/2^7$, $15/2^6$, $17/2^5$, $19/2^4$, $21/2^3$, $23/2^2$, 25/2, 27/2
	(5, 3/2)	1/2, $3/2^2$, $5/2^2$, $7/2^3$, $9/2^3$, $11/2^3$, $13/2^3$, $15/2^2$, $17/2^2$, 19/2, 21/2, 23/2

Table 3. Calculated magnetic moments of nuclei

	Configuration	$T=\|T_\zeta\|$	(s, t)	J	μ_{cal}	μ_{exp}
n		1/2		1/2		−1.91
H^1		1/2		1/2		2.79
H^3	$(s_{1/2})^{-1}$	1/2	(1, 1/2)	1/2	2.72	2.97
H^2	$(s_{1/2})^2$	0	(2, 0)	1	0.88	0.86
He^3	$(s_{1/2})^{-1}$	1/2	(1, 1/2)	1/2	−1.92	−2.13
Li^6	$(p_{3/2})^2$	0	(2, 0)	1	0.63	0.82
Li^7	$(p_{3/2})^3$	1/2	(1, 1/2)	3/2	3.07	3.26
Be^9	$(p_{3/2})^{-3}$	1/2	(1, 1/2)	3/2	−1.14	−1.18
B^{10}	$(p_{3/2})^{-2}$	0	(2, 0)	3	1.88	1.80
B^{11}	$(p_{3/2})^{-1}$	1/2	(1, 1/2)	3/2	3.79	2.69
C^{13}	$(p_{1/2})^1$	1/2	(1, 1/2)	1/2	0.64	0.70
N^{14}	$(p_{1/2})^2$	0	(2, 0)	1	0.37	0.40
N^{15}	$(p_{1/2})^{-1}$	1/2	(1, 1/2)	1/2	−0.27	−0.28
O^{17}	$(d_{5/2})^1$	1/2	(1, 1/2)	5/2	−1.91	−1.86
F^{19}	$(d_{5/2})^3$	1/2	(3, 1/2)	1/2	2.74	2.63
Ne^{21}	$(d_{5/2})^5$	1/2	(3, 3/2)	3/2	−0.65	<0
Na^{22}	$(d_{5/2})^6$	0	(6, 0)	3	1.73	1.75
Na^{23}	$(d_{5/2})^{-5}$	1/2	(3, 3/2)	3/2	2.38	2.22
Mg^{25}	$(d_{5/2})^{-3}$	1/2	(1, 1/2)	5/2	−0.62	−0.96
Al^{27}	$(d_{5/2})^{-1}$	1/2	(1, 1/2)	5/2	4.79	3.64
Si^{29}	$(s_{1/2})^1$	1/2	(1, 1/2)	1/2	−1.91	
P^{31}	$(s_{1/2})^{-1}$	1/2	(1, 1/2)	1/2	2.79	1.13
S^{33}	$(d_{3/2})^1$	1/2	(1, 1/2)	3/2	1.14	0.63
S^{35}	$(d_{3/2})^3$	3/2	(3, 3/2)	3/2	1.14	
Cl^{35}	$(d_{3/2})^3$	1/2	(1, 1/2)	3/2	0.26	0.82
Cl^{37}	$(d_{3/2})^{-3}$	3/2	(3, 3/2)	3/2	0.12	0.68
K^{39}	$(d_{3/2})^{-1}$	1/2	(1, 1/2)	3/2	0.12	0.39
K^{40}	$(d_{3/2})^{-1}(f_{7/2})^1$	1	(2, 1)	4	−1.70	−1.29
K^{41}	$(d_{3/2})^{-1}(f_{7/2})^2$	3/2	(1, 1/2)	3/2	0.12	0.22
Sc^{45}	$(f_{7/2})^5$	3/2	(1, 1/2)	7/2	5.07	4.8
V^{51}	$(f_{7/2})^{-5}$	5/2	(1, 1/2)	7/2	5.79	5.14
Mn^{55}	$(f_{7/2})^{-3}(f_{5/2})^2$	5/2	(3, 3/2)	5/2	4.1	3.47

Table 4. Predicted spins for some nuclei

Nuclei	Predicted Spin
Ne^{21}, Na^{23}	3/2, 9/2
Mn^{55}	3/2, 5/2, 9/2, 11/2, 15/2

Table 5. Magnetic moment of Mg^{25}

Configuration	T_z	(s, t)	μ_{cal}	μ_{exp}
$(d_{5/2})^3$	1/2	(1, 1/2)	−0.62	−0.96
		(3, 1/2)	2.3	

Table 6. Magnetic moment of Cl^{35}

configuration	T	μ_{cal}	μ_{exp}
$(d_{3/2})^3$	1/2	0.26	0.82
	3/2	0.80	

Table 7. Magnetic moments calculated by the assumption 1′

	Configration	$T=T_\zeta$	Spin	μ_{cal}	μ_{exp}
P^{31}	$(d_{3/2})^3$	1/2	1/2	0.72	1.13
S^{33}	$(d_{3/2})^{-3}$	1/2	3/2	1.00	0.63
Cl^{35}	$(d_{3/2})^{-1}$	1/2	3/2	0.12	0.82
Cl^{37}	$(d_{3/2})^{-1}(s_{1/2})^2$	3/2	3/2	0.12	0.68
K^{40}	$(s_{1/2})^{-1}(f_{7/2})^1$	1	4	0.85	−1.29

Table 8. Magnetic moments calculated by the assumption 1″

	Configuration	$T=T_\zeta$	J	μ_{cal}	μ_{exp}
P^{31}	$(s_{1/2})^1(d_{3/2})^2$	1/2	1/2	1.24	1.13
S^{33}	$(d_{3/2})^3(s_{1/2})^2$	1/2	3/2	0.92	0.63
Cl^{35}	$(d_{3/2})^{-3}(s_{1/2})^{-2}$	1/2	3/2	0.35	0.82
Cl^{37}	$(d_{3/2})^{-3}$	3/2	3/2	0.12	0.68
K^{39}	$(d_{3/2})^{-1}$	1/2	3/2	0.12	0.39
K^{40}	$(d_{3/2})^{-1}(f_{7/2})^{-1}$	1	4	−1.70	−1.29

Table 9. Beta-decay of mirror nuclei

	Configuration	$ft/10^3$
n	$(s_{1/2})^1$	1
H^3	$(s_{1/2})^{-1}$	1.1
C^{11}	$(p_{3/2})^{-1}$	3.9
N^{13}	$(p_{1/2})^1$	4.8
O^{15}	$(p_{1/2})^{-1}$	3.7
F^{17}	$(d_{5/2})^1$	2.2
Si^{27}	$(d_{5/2})^{-1}$	3.6
P^{29}	$(s_{1/2})^1$	3.8
S^{31}	$(s_{1/2})^{-1}$	3.4
Cl^{33}	$(d_{3/2})^1$	4.0
A^{35}	$(d_{3/2})^3$	3.4
Sc^{41}	$(f_{7/2})^1$	2.6

Table 10. Beta-decay of the nuclei which have the same configurations and spins as the final nuclei but are not mirror transitions

	Configuration	Log ft
S^{35}	$(d_{3/2})^3$	5.01
Sc^{43}	$(f_{7/2})^3$	4.81

Table 11. Beta-decay of the nuclei which have the same configurations as but spins different from the final nuclei

	Configuration	J_i	J_f	Log ft
Ne^{23}	$(d_{5/2})^5$	5/2	3/2	5.01
Na^{25}	$(d_{5/2})^{-3}$	3/2	5/2	4.8
Sc^{47}	$(f_{7/2})^7$	7/2	5/2	5.65

Table 12. Beta-decay of the type $j=l+1/2 \rightleftarrows j=l-1/2$

	Configuration	Log ft
B^{12}	$(p_{3/2})^{-1}(p_{1/2})^1$	4.18
N^{12}	$(p_{1/2})^1(p_{3/2})^{-1}$	4.18

Table 13. l-forbidden beta decay

	Configuration	Log ft
P^{32}	$(s_{1/2})^{-1}(d_{3/2})^1$	7.9

Table 14. j-seniority forbidden beta-decay

	si	sf	Log ft
Ca^{45}	5	1	5.98
Sc^{44}	4	0	>5.27

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Electronic States of F_2– and O_2–Molecules

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Electronic states of the F_2–molecule are first discussed on the basis of an assumption that the component F–atom is an ideal system which consists of five $2p$–electrons and a nucleus of charge $5e$ (the perfect screening by $1s$– and $2s$–electrons). The result of the calculation is that the ground state is $^1\Sigma_g^+$ and its dissociation energy and the corresponding equilibrium nuclear distance are 26.0 eV and 0.840×10^{-8} cm., respectively. Experiment shows that the ground state is $^1\Sigma_g^+$, the dissociation energy is smaller than 2.75 eV, and the corresponding equilibrium nuclear distance is 1.435×10^{-8} cm. The disagreement of the present result with experiment may be due to the neglect of the effect of s–electrons.

Next, we consider the electronic states of the O_2–molecule. In this case, we assume that the electron configuration of the O–atom is $1s^2 2s^2 2p\sigma 2p\pi^3$ and that $1s^2 2s^2 2p\sigma$ form "the molecular core." Thus we discuss the interaction between two ideal atoms each of which consists of three $2p\pi$ electrons and a nucleus. We find that the calculated result accounts for experiment.

Introduction

In the previous paper[1] (which will be referred to as "I" in what follows), we discussed the electronic states of C_2–molecules considering a system of two ideal atoms (C–atom) each consisting of two $2p$–electrons and a nucleus of double charges. We found a fact: "The more the $2p_\sigma$–electrons, the deeper the binding energy." This was due to the neglect of $2s$–electrons (and $1s$–electrons). When we took into account the effect of $2s$–electrons, we found that the rearrangement of the energy levels occurred.[2] The reason is as follows: The attractive force between a $2p_\sigma$–electron of an atom and a nucleus of the other is larger than that between a $2p_\pi$–electron and a nucleus, while the repulsive forces of s–electrons are stronger for p_σ–electrons than for p_π–electrons as is easily seen from the symmetry of the orbitals.

In the present paper we first consider the interaction between two F–atoms which consist respectively of five $2p$–electrons and a nucleus of charge $5e$. We arrive at the same conclusion as in I, that is, the configurations which contain more p_σ–electrons have the lower energy. Thus, we have to take into account the interaction between $2p_\sigma$ and $2s$ electrons.

In the case of F_2–molecules, however, the calculation including $2s$–electrons is extremely lengthy and tedious. A more simplified method of treating the molecules are hence desired to device. The neglect of $2p_\sigma$ as well as $2s$ electrons can be a tentative way. It is imagined that this method gives rather a better result. In such a direction we hit upon three models:

(i) We assume $1s^2 2s^2 2p_\sigma^2 2p_\pi^3$ for the electron configuration of an F–atom. We consider $1s^2 2s^2 2p_\sigma^2$ as to form "the molecular core," and neglect them altogether. We have then only to consider the interaction between two ideal atoms containing three $2p_\pi$ electrons each.

(ii) We assume $1s^2 2s^2 2p_\sigma 2p_\pi^4$ for the electron configuration of an F–atom. We consider $1s^2 2s^2 2p_\sigma$ as "the molecular core." In this case the F_2–molecule consists of two atoms which contain four $2p_\pi$ electrons each.

(iii) The configuration of an F–atom is as in (ii) and we neglect $1s^2 2p_\pi^4$. The F_2–molecule becomes a system of consisting of two atoms which contain two $2s$–electrons and one $2p_\sigma$–electron each.

To determine in purely theoretical way which of these models is the better approximation is impossible unless we take into account completely all electrons. If we adopt the model (ii), the electronic state of a F_2–molecule is only $(\pi^2\bar{\pi}^2, \pi^2\bar{\pi}^2)^1\Sigma_g^+$. And if the adiabatic potential of this state is attractive, we have to consider this state to be the ground state of F_2. This way is equivalent to the molecular orbital method. If we take the model (i), electronic states of a F_2–molecule are $^3\Delta_u$, $^1\Delta_g$, $^3\Sigma_g^-$, $^3\Sigma_u^+$, $^1\Sigma_g^+$, and $^1\Sigma_u^-$ as we discuss in the case of O_2–molecules. It seems that among the adiabatic potential of these six states that of $^3\Sigma_g^-$ state is lowest, and we can not explain the experimental fact in which the ground state is $^1\Sigma_g^+$. As for the model (iii) we hope to consider it more precisely elsewhere. The electronic states of this model are all Σ. It is experimentally believed that the deepest state of the F_2–molecule is $^1\Sigma_g^+$ and next and third are Π states.

We next discuss the electronic states of O_2–molecules. They have qualitatively been discussed by many authors.[3] A quantitative theory was first published by Wheland.[4] He assumed $1s^2 2s^2 2p_\sigma 2p_\pi^3$ for the electron configuration of the O–atom and neglected $1s$– and $2s$–electrons. He regarded two $2p_\sigma$ electrons as forming a single bond and ignored their interaction with the remaining electrons. Thus he treated six $2p_\pi$ electron system (three in each atom) and found that the $^3\Sigma_g^-$ state was the lowest of the states arising from this configuration. From this result he drew a conclusion that the $^3\Sigma_g^-$ state might be the ground state of the O_2–molecule.

In the present paper we assume the same electron configuration of the O–atom as Wheland, because this assumption can be considered as quite natural from the result obtained in II. The configuration $1s^2 2s^2 2p_\sigma$ is considered as the molecular core as before, and the electronic states of the O_2–molecule is discussed considering the interaction of two ideal atoms which contain three $2p_\pi$–electrons each. The calculated result for energy values shows that the lowest state is $^3\Sigma_g^-$, which is in agreement with experiment. The excitation energy and symmetry properties of lower three excited states are in agreement with experiment.

The method of calculation and the notations for various orbitals, wave functions and integrals are the same as I and II throughout in the present paper. Numerical evaluation is carried out by making use of the tables given in III.[5] Orbitals are denoted by

$$\sigma = N_z \cdot Z \cdot \exp(-\varkappa r/2),$$

$$\pi = N_\pi (x+iy)\exp(-\varkappa r/2), \quad \varphi = N_\pi (x-iy)\exp(-\varkappa r/2).$$

§ 1. F_2-molecules

The electronic part of the Hamiltonian of our ideal F-molecule is given by

$$H = -\sum_{k=1}^{10}\left(\frac{1}{2}\Delta_k + \frac{5}{r_{ak}} + \frac{5}{r_{bk}}\right) + \sum_{k=j+1}^{10}\sum_{j=1}^{10}\frac{1}{r_{jk}} + \frac{25}{R}$$

where all quantities are measured in atomic units. If we neglect the effect of the excited and ionic structures, the electronic states arising from various configurations of the molecule are as follows:

Λ	*configurations*	*states*	*wave functions*
2	$(\sigma^2\pi^2\varphi, \sigma^2\pi^2\varphi)$	$^3\Delta_u$	$(\sigma_a^+\sigma_a^-\pi_a^+\pi_a^-\varphi_a^+\sigma_b^+\sigma_b^-\pi_b^+\pi_b^-\varphi_b^+)$
		$^1\Delta_g$	$(\sigma_a^+\sigma_a^-\pi_a^+\pi_a^-\varphi_a^+\sigma_b^+\sigma_b^-\pi_b^+\pi_b^-\varphi_b^-) - (\sigma_a^+\sigma_a^-\pi_a^+\pi_a^-\varphi_a^-\sigma_b^+\sigma_b^-\pi_b^+\pi_b^-\varphi_b^+)$
1	$(\sigma^2\pi^2\varphi, \sigma\pi^2\varphi^2)$	$^3\Pi_{g,u}$	$(\sigma_a^+\sigma_a^-\pi_a^+\pi_a^-\varphi_a^+\sigma_b^+\pi_b^+\pi_b^-\varphi_b^+\varphi_b^-) \mp (\sigma_a^+\pi_a^+\pi_a^-\varphi_a^+\varphi_a^-\sigma_b^+\sigma_b^-\pi_b^+\pi_b^-\varphi_b^+)$
		$^1\Pi_{g,u}$	$(\sigma_a^+\sigma_a^-\pi_a^+\pi_a^-\varphi_a^+\sigma_b^-\pi_b^+\pi_b^-\varphi_b^+\varphi_b^-) \pm (\sigma_a^+\pi_a^+\pi_a^-\varphi_a^+\varphi_a^-\sigma_b^+\sigma_b^-\pi_b^+\pi_b^-\varphi_b^-)$
			$\mp (\sigma_a^-\pi_a^+\pi_a^-\varphi_a^+\varphi_a^-\sigma_b^+\sigma_b^-\pi_b^+\pi_b^-\varphi_b^+) - (\sigma_a^+\sigma_a^-\pi_a^+\pi_a^-\varphi_a^-\sigma_b^+\pi_b^+\pi_b^-\varphi_b^+\varphi_b^-)$
0	$(\sigma^2\pi^2\varphi, \sigma^2\pi\varphi^2)$	$^3\Sigma_g^-$, $^3\Sigma_u^+$	$(\sigma_a^+\sigma_a^-\pi_a^+\pi_a^-\varphi_a^+\sigma_b^+\sigma_b^-\pi_b^+\varphi_b^+\varphi_b^-) \mp (\sigma_a^+\sigma_a^-\pi_a^+\varphi_a^+\varphi_a^-\sigma_b^+\sigma_b^-\pi_b^+\pi_b^-\varphi_b^+)$
		$^1\Sigma_g^+$, $^1\Sigma_u^-$	$(\sigma_a^+\sigma_a^-\pi_a^+\pi_a^-\varphi_a^+\sigma_b^+\sigma_b^-\pi_b^-\varphi_b^+\varphi_b^-) - (\sigma_a^+\sigma_a^-\pi_a^+\pi_a^-\varphi_a^-\sigma_b^+\sigma_b^-\pi_b^+\varphi_b^+\varphi_b^-)$
			$\mp (\sigma_a^+\sigma_a^-\pi_a^-\varphi_a^+\varphi_a^-\sigma_b^+\sigma_b^-\pi_b^+\pi_b^-\varphi_b^+) \pm (\sigma_a^+\sigma_a^-\pi_a^+\varphi_a^+\varphi_a^-\sigma_b^+\sigma_b^-\pi_b^+\pi_b^-\varphi_b^-)$
	$(\sigma\pi^2\varphi^2, \sigma\pi^2\varphi^2)$	$^3\Sigma_u^+$	$(\sigma_a^+\pi_a^+\pi_a^-\varphi_a^+\varphi_a^-\sigma_b^+\pi_b^+\pi_b^-\varphi_b^+\varphi_b^-)$
		$^1\Sigma_g^+$	$(\sigma_a^+\pi_a^+\pi_a^-\varphi_a^+\varphi_a^-\sigma_b^-\pi_b^+\pi_b^-\varphi_b^+\varphi_b^-) - (\sigma_a^-\pi_a^+\pi_a^-\varphi_a^+\varphi_a^-\sigma_b^+\pi_b^+\pi_b^-\varphi_b^+\varphi_b^-)$

where Λ is the axial quantum number of the molecule.

We first calculate the expectation values of H with respect to the above mentioned states: $W=(\psi, H\psi)/(\psi, \psi)$ where ψ denotes the wave function of the state in question. The result of the calculation for $\varkappa=5$ and $1.4 \leq R \leq 2.0$ is plotted in Fig. 1. We can find, from this figure, the rough order of these 12 electronic states. The lowest level is either $(\sigma^2\pi^2\varphi, \sigma^2\pi\varphi^2)^1\Sigma_g^+$ or $(\sigma^2\pi^2\varphi, \sigma^2\pi^2\varphi)^1\Delta_g$. The $^1\Sigma_g^+$ state, however, also arises from the configuration $(\sigma\pi^2\varphi^2, \sigma\pi^2\varphi^2)$ and the interaction between these two $^1\Sigma_g^+$ states lowers the adiabatic potential curve of $(\sigma^2\pi^2\varphi, \sigma^2\pi\varphi^2)^1\Sigma_g^+$ state. It seems therefore that the ground state of the molecule is $(\sigma^2\pi^2\varphi, \sigma^2\pi\varphi^2)^1\Sigma_g^+$.

Now, we shall examine the $^1\Sigma_g^+$ states in detail. This state arises from $(\sigma^2\pi^2\varphi, \sigma^2\pi\varphi^2)$ and $(\sigma\pi^2\varphi^2, \sigma\pi^2\varphi^2)$. The secular equation which determines the energy of the state is of the 2nd degree. The method of calculating the energy was explained in detail in II. The effective charge $\varkappa$ is considered as the function of R and the variational method is applied to the calculation. The numerical evaluation is carried out by making use of the tables given in III. We get 0.960 atomic units = 26.0 eV for the dissociation energy

of $^1\sum_g^+$ state and $R_{\min}=1.59$ atomic units$=0.84$ Å for the corresponding equilibrium nuclear distance. The corresponding effective charge is 3.62. The numerical evaluation shows that the contribution from the configuration $(\sigma\pi^2\bar{\pi}^2, \sigma\pi^2\bar{\sigma}^2)$ is very small.

The experimentally determined ground state of the F_2–molecule[6] is $(\sigma\pi^2\bar{\pi}^2, \sigma\pi^2\bar{\sigma}^2)\ ^1\sum_g^+$. The observed value of the dissociation energy is smaller than 2.75 eV and the corresponding equilibrium nuclear distance is 1.435 Å. The above obtained result of the present calculation is by no means in agreement with these observed facts. The reason for this disagreement is the neglect of the $2s$– (and $1s$–) electrons. The strong attractive force between the σ–electron of one of the two atoms and a nucleus of the other is the source of the main contribution to the binding energy. If we take into account the effect of $2s$–electrons, the strong repulsive force between $2s$ and $2p_\sigma$–electrons may cancel most of the attractive force. The dissociation energy may consequently become far smaller, and the equilibrium nuclear distance longer. This is naturally expected from the fact found in II. Since the interaction between $2s$ and $2p_\pi$–electron is very small, it may be also natural to expect that the ground state of the F_2–molecule is $(s^2\sigma\pi^2\bar{\pi}^2, s^2\sigma\pi^2\bar{\sigma}^2)\ ^1\sum_g^+$.

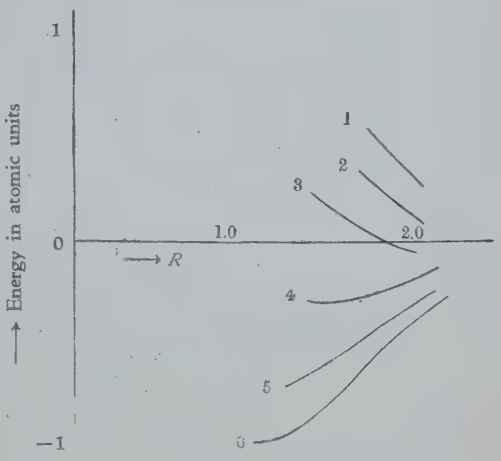

Fig. 1 Adiabatic potentials of F_2–molecule.
R: nuclear distance in atomic units.
1) $(\sigma\pi^2\bar{\pi}^2, \sigma\pi^2\bar{\sigma}^2)\ ^3\sum_u^+$,
2) $(\sigma^2\pi^2\bar{\pi}^2, \sigma^2\pi\bar{\sigma}^2)\ ^3\sum_g^+$, $(\sigma\pi^2\bar{\pi}^2, \sigma\pi^2\bar{\sigma}^2)\ ^1\sum_g^+$,
3) $(\sigma^2\pi^2\bar{\pi}^2, \sigma\pi^2\bar{\sigma}^2, ^3, ^1\Pi_u$,
4) $(\sigma^2\pi^2\bar{\pi}^2, \sigma\pi^2\bar{\sigma}^2, ^3, ^1\Pi_g$,
5) $(\sigma^2\pi^2\bar{\pi}^2, \sigma^2\pi^2\bar{\pi}^2, ^3\Delta_u$, $(\sigma^2\pi^2\bar{\pi}^2, \sigma^2\pi\bar{\sigma}^2, ^3\sum_u^+, ^1\sum_u^-$,
6) $(\sigma^2\pi^2\bar{\pi}^2, \sigma^2\pi^2\bar{\pi}^2)\ ^1\Delta_g$, $(\sigma^2\pi^2\bar{\pi}^2, \sigma^2\pi\bar{\sigma}^2)\ ^1\sum_g^+$.

§ 2. O_2–molecules

We consider next the electronic states of the O_2–molecules in this section. We neglect $1s^2 2s^2 2p_\sigma$ electrons altogether. The Hamiltonian is given in the similar way as in the F_2–molecule:

$$H=-\sum_{i=1}^{6}\left(\frac{1}{2}\Delta_i+\frac{3}{r_{ai}}+\frac{3}{r_{bi}}\right)+\sum_{k=i+1}^{6}\sum_{i=1}^{6}\frac{1}{r_{ik}}+\frac{9}{R}\ .$$

In such a rough approximation we can not plot the adiabatic potential and we can accordingly not discuss the dissociation energy and the equilibrium nuclear distance. The electronic states arising from the configuration which consists of six $2p_\pi$ electrons are, as follows:

Λ	*configurations*	*states*	*wave functions*
2	$(\pi^2\bar{\sigma}, \pi^2\bar{\sigma})$	$^3\Delta_u$	$(\pi_a^+\pi_a^-\bar{\sigma}_a^+\pi_b^+\pi_b^-\bar{\sigma}_b^+)$
		$^1\Delta_g$	$(\pi_a^+\pi_a^-\bar{\sigma}_a^+\pi_b^+\pi_b^-\bar{\sigma}_b^-) - (\pi_a^+\pi_a^-\bar{\sigma}_a^-\pi_b^+\pi_b^-\bar{\sigma}_b^+)$
0	$(\pi^2\bar{\sigma}, \pi\bar{\sigma}^2)$	$^3\Sigma_g^-$, $^3\Sigma_u^+$	$(\pi_a^+\pi_a^-\bar{\sigma}_a^+\pi_b^+\bar{\sigma}_b^+\bar{\sigma}_b^-) \mp (\pi_a^+\bar{\sigma}_a^+\bar{\sigma}_a^-\pi_b^+\pi_b^-\bar{\sigma}_b^+)$
		$^1\Sigma_g^+$, $^1\Sigma_u^-$	$(\pi_a^+\pi_a^-\bar{\sigma}_a^+\pi_b^-\bar{\sigma}_b^+\bar{\sigma}_b^-) - (\pi_a^+\pi_a^-\bar{\sigma}_a^-\pi_b^+\bar{\sigma}_b^+\bar{\sigma}_b^-)$ $\mp (\pi_a^-\bar{\sigma}_a^+\bar{\sigma}_a^-\pi_b^+\pi_b^-\bar{\sigma}_b^+) \pm (\pi_a^+\bar{\sigma}_a^+\bar{\sigma}_a^-\pi_b^+\pi_b^-\bar{\sigma}_b^-)$

Hence the degrees of the secular equations are all linear, and the energy W of each state is simply given by the expectation value of the Hamiltonian. The result of the calculation is given by the following equations:

$$W(^1\Sigma_g^+) = W(^1\Delta_g) - W_1\,, \quad W(^1\Sigma_u^-) = W(^3\Delta_u) - W_2\,,$$
$$W(^3\Sigma_g^-) = W(^1\Delta_g) + W_1\,, \quad W(^3\Sigma_u^+) = W(^3\Delta_u) + W_2\,.$$

where

$$W(^1\Delta_g) = \frac{A-B}{a-b}\,, \qquad W(^3\Delta_u) = \frac{A+B}{a+b}\,,$$
$$W_1 = \frac{C-D}{a-b}\,, \qquad W_2 = \frac{C+D}{a+b}\,,$$
$$A = ((\pi_a^+\pi_a^-\bar{\sigma}_a^+\pi_b^+\pi_b^-\bar{\sigma}_b^-),\ H(\pi_a^+\pi_a^-\bar{\sigma}_a^+\pi_b^+\pi_b^-\bar{\sigma}_b^-))\,,$$
$$B = ((\pi_a^+\pi_a^-\bar{\sigma}_a^+\pi_b^+\pi_b^-\bar{\sigma}_b^-),\ H(\pi_a^+\pi_a^-\bar{\sigma}_a^-\pi_b^+\pi_b^-\bar{\sigma}_b^+))\,,$$
$$C = -C_{\pi\bar{\sigma}\cdot\bar{\sigma}\pi}((1+S_1^2)^2 + 4L_{\pi\bar{\sigma}\cdot\bar{\sigma}\pi}S_1^2(1+S_1^2)^2 - 2(F_{\pi\bar{\sigma}\cdot\bar{\sigma}\pi} + D_{\pi\bar{\sigma}\cdot\bar{\sigma}\pi}S_1^2\,,$$
$$D = D_{\pi\bar{\sigma}\cdot\bar{\sigma}\pi}(1+S_1^4) + 2F_{\pi\bar{\sigma}\cdot\bar{\sigma}\pi}S_1^2 - 4L_{\pi\bar{\sigma}\cdot\bar{\sigma}\pi}S_1(1+S_1^2) + 4C_{\pi\bar{\sigma}\cdot\bar{\sigma}\pi}S_1^2\,,$$
$$a = (1-S_1^2)^2\,, \qquad b = -S_1^2\cdot a\,.$$

Numerical values of $C/\varkappa$ and $D/\varkappa$ are easily obtained as the function of $\varkappa R$ by making use of the tables given in III. We find that

$$W_1 < 0\,, \qquad W_2 < 0\,.$$

In Fig. 2 the values of W_1 and W_2 are plotted as the functions of R for $\varkappa = 3$. The integrals A and B are reduced and evaluated in the manner explained in detail in II, and we get the followlng relation:

$$W(^3\Delta_u) > W(^1\Delta_g) \quad \text{for} \quad \varkappa = 3 \quad \text{and} \quad \varkappa R < 9\,.$$

It can be inferred that this relation may be satisfied in the larger domain. $W(^1\Delta_g) - W(^3\Delta_u)$ is of the order of $10\,W_1$ or $10\,W_2$. The curves of $W(^3\Delta_u)$, $W(^1\Delta_g)$ and $W(^3\Delta_u) - W(^1\Delta_g)$ are plotted in Fig. 2. Since the observed value of the equilibrium nuclear distance of the O_2-molecule is about $2.0 \sim 2.5$ atomic units in its lower electronic states, it is sufficient to consider the energy value in the domain $\varkappa R < 9$. From the above-mentioned inequality relations we can conclude that the ground state of the O_2-molecule is $^3\Sigma_g^-$. Moreover, if we take $\varkappa = 3$, in the range $6 \leq R \leq 7$ we have

$$W(^3\Delta_u) - W(^1\Delta_g) \sim 0.2\,; \quad W_1 \sim W_2 \sim 0.02\,.$$

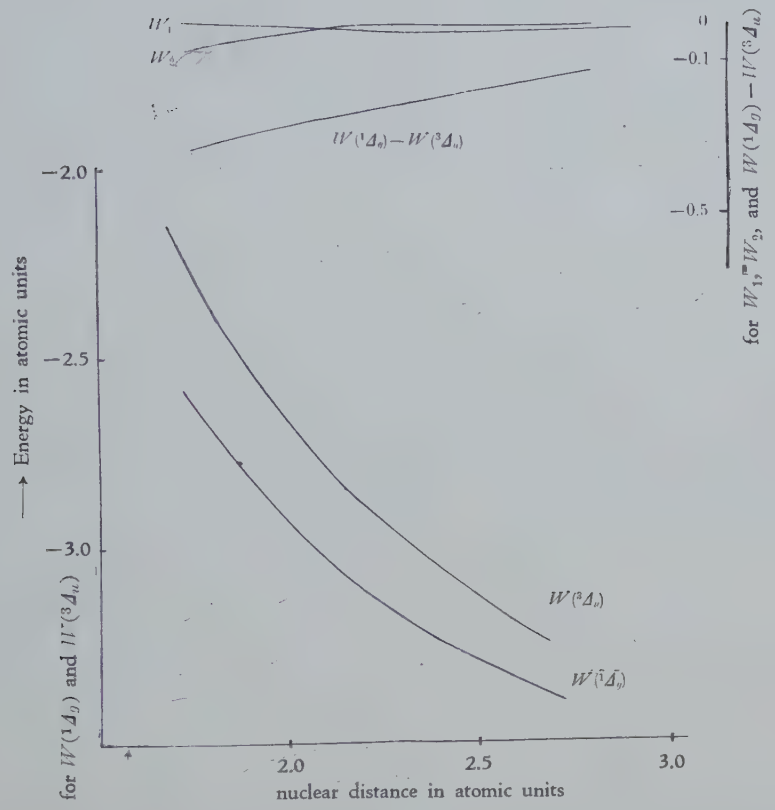

Fig. 2. Curves of W_1, W_2, $W(^3\Delta_u)$, $W(^1\Delta_g)$ and $W(^3\Delta_u)-W(^1\Delta_g)$ as the fuctions of R for $\varkappa=3$.

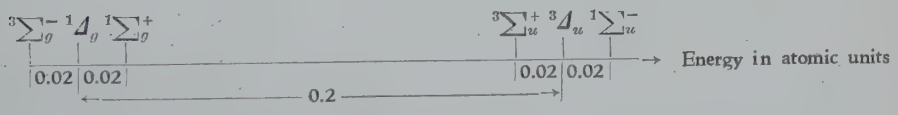

Fig. 3 Schematic representation of the results for the O_2–molecule.

The quantitative relation between above mentioned states is shown schematically in Fig. 3.

The experimental results[6] for the O_2–molecules are as follows: The ground state is $^3\sum_g^-$, lower four excited states are $^1\Delta_g$, $^1\sum_g^+$, $^3\sum_u^+$, and $^3\sum_u^+$ in order of increasing energy. The energy intervals between ground $^3\sum_g^-$ state and $^1\Delta_g$, $^1\sum_g^+$, and $^3\sum_u^+$ are 0.98 eV ($\sim$0.036 a.u.), 1.63 eV ($\sim$0.060 a.u.) and 4.47 eV ($\sim$0.165 a.u.) respectively. The agreement between the theoretically estimated and observed values are very good.

The electrons which are contained in the ignored cores are all s or σ. The interaction of these electrons with $2p_\pi$ electrons are very small and all similar in character. The electronic state of "the molecular core" may be $^1\sum_g^+$. Therefore it may be inferred that

the effects of ignoring core do not alter the above-mentioned theoretical result. The ionic configuration which may affect the result are $(\pi^2\bar{\pi}^2, \pi^2)^1\Delta_u$ and $(\pi^2\bar{\pi}^2, \pi\bar{\pi})^3\Sigma_g^-$, $^1\Sigma_u^+$. The influence of these states are very small and the shifts of energy levels of $^1\Delta_g$ and $^3\Sigma_g^-$ may be smaller than 0.01 a.u. which is negligible in our consideration.

The present assumption may of course be adequate only for a few states near the ground state, and we must consider the effects of the excited atomic configulations for higher levels, for example, the observed $^3\Sigma_u^-$ state may be $(\pi^2\bar{\pi}^2, \pi\bar{\pi})^3\Sigma_u^-$. That the experimental values of intervals $^1\Delta_g - {}^3\Sigma_u^-$ and $^1\Sigma_g^+ - {}^1\Delta_g$ are not equal may also be due to the effect of ionic configurations. If we treated the electronic states of O_2–molecules in the similar manner as F_2–molecules in the first section or C_2–molecules in I, we would obtain the unsatisfactory result as before.

In conclusion the author wishes to express his sincere thanks to Professor Gentaro Araki for the valuable suggestions and encouragement he has given in the course of the present work.

References

1) G. Araki, S. Tutihasi and W. Watari, Prog. Theor. Phys. **6** (1951), 135, this is referred to as I.
2) G. Araki and W. Watari, Prog. Theore. Phys. **6** (1951), 945, this is referred to as II.
3) J. E. Lennard-Jones, Trans. Faraday Soc. **25** (1929), 668.
R. S. Mulliken, Rev. Mod. Phys. **4** (1934), 1.
W. Heitler and G. Pöschl, Nature **133** (1934), 833.
W. Moffitt, Proc. Royal Soc. **A210** (1951), 224.
4) G. W. Wheland, Trans. Faraday Soc. **33** (1937), 1499.
5) G. Araki and W. Watari, Prog. Theor. Phys. **6** (1651), 961, this is referred to as III.
6) G. Herzberg, "*Molecular Spectra and Molecular Structure I*" (D. Van Nostrand Company) 2nd ed. (1950).

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Pion Reactions in One Nucleon System and Nucleon Isobars

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In this paper, we try to interpret the pion-nucleon interaction on the basis of the nucleon isobar model. As a complementary way to the strong coupling and phenomenological theories, we start from the field theoretical viewpoint which will be useful to connect the present phenomenological theory of pions to the future theory of fields.

We treat the nucleon isobars as elementary particles and describe them by the Rarita-Schwinger equation of particles with spin 3/2. Hence the familiar Feynman-Dyson method is immediately applicable to the calculation of matrix elements of such processes involving nucleon isobars as the pion-proton scattering and the pion-production by γ-rays on proton.

The qualitative features are governed mainly by the mass, width, spin and isotopic spin of the isobar, so that our results roughly agree with those of the strong coupling and phenomenological theories.

In some detailed respects, however, our results show differences from other theories; the agreement with experiments is improved for the angular distributions of $\pi-p$ scattering and photo-production of charged pions, but becomes a little worse for that of neutral pions.

Our method is applied only to pion reactions in one nucleon system, for we know too little about two or more nucleon systems to extract the pure pion-nucleon interaction. Lastly, we discuss the validity of the nucleon isobars.

§ 1. Introduction

The queer behaviour of pions can hardly be understood in terms of the lowest order perturbation theory in contrast to the case of quantum electrodynamics, and various methods such as the higher order calculations, strong coupling and phenomenological theories are occasionally employed to account for experimental results.

None of the methods thus far employed has given a satisfactory agreement with experiments, but each of them may correspond to a part of truth. In the phenomenological theory there are a number of quantities which correspond directly to observed ones, but are introduced without further verification.

The strong coupling theory can give such phenomenological quantities, but seems to be based upon idealized assumptions and crude approximations which may not be permitted. Among those which are in doubt is the assumption of infinitely heavy nucleons. Then the recoil of nucleons and the radiative corrections are inevitably discarded. These dis-

advantageous points may more or less be remedied in the perturbation theory with higher order corrections, but the actual computation is too laborious to be performed.

Taking merits of the above theories, we propose a method which can take account of the recoil and a part of higher order effects as well as of the strong coupling nature of pions that gives rise to the isobar state. This is to treat the nucleon in an isobar state, as if it were an elementary particle of spin 3/2 that obeys the Rarita-Schwinger equation.[1] Its interactions with other fields are introduced within the frame of the canonical formalism. Such a fictitious elementary particle appears only in intermediate states of the perturbation calculation, to which the relativistic method can be applied with the aid of the propagation function for a spin 3/2 particle, as described in Part I.

Also in this treatment, there exists such oversimplification as to replace the complicated higher order interaction between a nucleon and a pion by a point interaction which is described by that between the fictitious particle and a pion. The meaning and validity of our method are discussed in Part IV and it is found that our method seems superior to others in many respects.

Our method is applied only to such processes that only one nucleon takes part in, avoiding the complication which arises from nucleon-nucleon interactions. The processes which we investigated are the pion-proton scattering (Part II) and the photo-pion production (Part III). The results agree with experiments better than in previous existing methods. The causes of disagreements are discussed on account of our approximation.

Part I. Nucleon Isobars

§ 2. Experimental implications of the existence of nucleon isobars

The existence of nucleon isobars was first suspected when the experimental results on the photo-pion production[2] showed the two reactions,

$$\gamma+p\rightarrow n+\pi^{+}, \tag{1}$$

$$\gamma+p\rightarrow p+\pi^{0} \tag{2}$$

being of a comparable order of cross sections at a photon energy of 300 Mev., whereas the lowest order perturbation theory predicts

$$\sigma^{0}/\sigma^{+}\sim(\mu/m)^{2},$$

where σ^{+} and σ^{0} are the cross sections of the reactions (1) and (2), and μ and m denote the rest masses of pion and nucleon respectively.

In order to get rid of this discrepancy, various ideas were proposed, e.g., several authors attempted to take into account the Pauli-type interaction between a nucleon and the electromagnetic field.[3]

However, since the theoretical value of σ^{0} was still lower than the one observed, several authors attacked the problem by assuming the existence of nucleon isobar[4] which is one of the most characteristic features of the strong coupling theory.

Recent experiments on the pion-proton scattering also showed an indication in favour of the isobar hypothesis.[6]

Assuming the existence of isobars, the excitation energy, width, spin and isotopic spin of the isobar are fixed in reference to the following experimental facts.

From the photo-production of neutral pions, it is already known that the excitation energy ΔE is about 240～300 Mev. and the width Γ about 60 Mev.*). The same isobaric state seems to contribute also to the pion-proton scattering*) and we shall identify them.

In the symmetrical theory, the isotopic spin is a good quantum number,**) with which we can provide an isobar and the isotopic spin of the isobar reveals itself as the most characteristic quantity in the pion-proton scattering.

The experimental results show

$$\sigma^+ : \sigma^- : \sigma^0 \approx 9 : 1 : 2$$

at energies about 110～150 Mev. where the resonance phenomena are supposed to take place.

The notations σ^+, σ^- and σ^0 represent the cross sections of the following modes of the pion-nucleon scattering :

$$\pi^+ + p \rightarrow p + \pi^+,$$
$$\pi^- + p \rightarrow p + \pi^-,$$
$$\pi^- + p \rightarrow n + \pi^+.$$

From the charge ratio, we know that only the states with the isotopic spin $I=3/2$ contribute dominantly to the scattering at resonance energies, so that we have to offer the value $I=3/2$ for the isotopic spin of the isobar.

Experiments on various pion reactions show that the pion interacts with nucleon strongly in P-states of orbital angular momentum, e.g., the excitation function of the photo-production of neutral pions near threshold, and the angular distribution of the produced positive pions in proton-proton collisions.[8]

The largeness of the total cross sections and the singular behaviour of the angular distributions in the pion-proton scattering also indicate the strong interaction in $P_{3/2}$ states in conformity with the above facts. Hence, we assume the spin J of the isobar to be equal to 3/2.

It is interesting to note that $I=3/2$ and $J=3/2$ are the natural consequences of the strong coupling theory.[9]

§ 3. The Rarita-Schwinger theory of particles with spin 3/2

In order that we are able to compute the matrix elements of processes involving

---

* These values are estimated from the resonance-like excitation functions of the reactions.

** We assume the symmetrical theory throughout this paper. The phase shift analysis of the pion-proton scattering indicates that the isotopic spin is a good quantum number.[7]

nucleon isobars, it is necessary to settle the field equation, propagation function and interaction scheme of the nucleon isobar.

As the field equation of the isobar, we shall adopt here the Rarita-Schwinger equation, for which the interaction with the electromagnetic field can consistently be introduced.

The Lagrangian of the Rarita-Schwinger field is given by

$$\mathfrak{L}=\bar{\Psi}_\mu(\gamma\partial+M)\Psi_\mu-\frac{1}{3}\bar{\Psi}_\mu(\gamma_\mu\partial_\nu+\gamma_\nu\partial_\mu)\Psi_\nu+\frac{1}{3}\bar{\Psi}_\mu\gamma_\mu(\gamma\partial-M)\gamma_\nu\Psi_\nu, \quad (3\cdot1)$$

from which follows, by means of the variation principle,

$$D_{\mu\nu}(\partial)\Psi_\nu=0, \quad (3\cdot2)$$

where

$$D_{\mu\nu}(\partial)=(\gamma\partial+M)\delta_{\mu\nu}-\frac{1}{3}(\gamma_\mu\partial_\nu+\gamma_\nu\partial_\mu)+\frac{1}{3}\gamma_\mu(\gamma\partial-M)\gamma_\nu. \quad (3\cdot3)$$

From (3·2) and (3·3), result immediately

$$\gamma_\mu\Psi_\mu=0, \quad \partial_\mu\Psi_\mu=0 \text{ and } (\gamma\partial+M)\Psi_\mu=0, \quad (3\cdot4)$$

because of the following algebraic relations:

$$\begin{aligned} &d_\rho D_{\rho\nu}=\partial_\nu, \quad d_\rho\equiv(1/M)\{\partial_\rho-(\gamma\partial)\gamma_\rho\}, \\ &\Gamma_\rho D_{\rho\nu}=\gamma_\nu, \quad \Gamma_\rho\equiv(1/M)(2d_\rho-3\gamma_\rho). \end{aligned} \quad (3\cdot5)$$

Inserting (3·5) into (3·3), we arrive at

$$D_{\mu\nu}=(\gamma\partial+M)\delta_{\mu\nu}-\frac{1}{3}[(\gamma_\mu d_\rho+\partial_\mu\Gamma_\rho)-\gamma_\mu(\gamma\partial-M)\Gamma_\rho]D_{\rho\nu},$$

i.e.,

$$(\gamma\partial+M)\delta_{\mu\nu}=[\delta_{\mu\rho}+\frac{1}{3}(\gamma_\mu d_\rho+\partial_\mu\Gamma_\rho)-\frac{1}{3}\gamma_\mu(\gamma\partial-M)\Gamma_\rho]D_{\rho\nu}.$$

Define

$$\mathfrak{S}_{\mu\rho}(\partial)=(\gamma\partial-M)\left[\delta_{\mu\rho}+\frac{1}{3}(\gamma_\mu d_\rho+\partial_\mu\Gamma_\rho)-\frac{1}{3}\gamma_\mu(\gamma\partial-M)\Gamma_\rho\right], \quad (3\cdot6)$$

then we have

$$D_{\lambda\rho}(\partial)\mathfrak{S}_{\rho\mu}(\partial)=\delta_{\lambda\mu}(\Box^2-M^2). \quad (3\cdot7)$$

Consequently the expression

$$\mathfrak{S}_F(x)=\mathfrak{S}(\partial)\Delta_F(x) \quad (3\cdot8)$$

plays the rôle of the propagation function in the Rarita-Schwinger theory.

§ 4. Interaction Lagrangians

We shall, next, study the properties of the interaction of the isobar with other fields. In order to interpret the resonance phenomena which take place in the pion-proton scattering, we have to introduce the interaction that causes

$$\pi+N\rightarrow\mathfrak{N}. \quad (N: \text{nucleon}, \mathfrak{N}: \text{isobar}) \tag{4·1}$$

Similarly we necessitate as well the interaction that gives rise to

$$\gamma+N\rightarrow\mathfrak{N}. \tag{4·2}$$

Since the isotopic spin I of the isobar is equal to $3/2$, the third component I_3 assumes the values $3/2$, $1/2$, $-1/2$, $-3/2$ corresponding to the four states with charge $2e$, e, 0, $-e$.

We shall denote these isobaric states as

$$\mathfrak{N}_2, \mathfrak{N}_1, \mathfrak{N}_0, \mathfrak{N}_{-1}. \tag{4·3}$$

The charge dependence of the interaction (4·1) must be expressed as

$$\mathfrak{L}_{int}\sim G_{ijk}\mathfrak{N}_i^* N_j \pi_k+\text{comp. conj.} \tag{4·4}$$

The requirement of charge independence can fix the form of G_{ijk} and (4·4) becomes as*)

$$\mathfrak{L}_{int}\sim G\Big[\mathfrak{N}_2^* p\pi^+-\frac{1}{\sqrt{3}}\mathfrak{N}_1^*(n\pi^+ +\sqrt{2}\,p\pi^0) +\frac{1}{\sqrt{3}}\mathfrak{N}_0^*(p\pi^- +\sqrt{2}\,n\pi^0)-\mathfrak{N}_{-1}^* n\pi^-\Big]+\text{comp. conj.} \tag{4·5}$$

or written more rigorously in the form of quantized operators, furnishes us with

$$\mathfrak{L}_{int}\sim G\Big[\bar{\Psi}_{(2)}\psi_P\phi-\frac{1}{\sqrt{3}}\bar{\Psi}_{(1)}(\psi_N\phi+\sqrt{2}\,\psi_P\phi_3) +\frac{1}{\sqrt{3}}\bar{\Psi}_{(0)}(\psi_P\phi^*+\sqrt{2}\,\psi_N\phi_3)-\bar{\Psi}_{(-1)}\psi_N\phi^*\Big]+\text{comp. conj.} \tag{4·6}$$

The interaction Lagrangians causing (4·1) and (4·2) are given apart from charge dependences by

$$\mathfrak{L}_1=-\frac{G}{\mu}\bar{\Psi}_\lambda O\psi\cdot\frac{\partial\phi}{\partial x_\lambda}+\text{comp. conj.}, \tag{4·7}$$

$$\mathfrak{L}_2=-i\frac{e}{m}\bar{\Psi}_\lambda\gamma_\mu O'\psi\cdot F_{\lambda\mu}+\text{comp. conj.}, \tag{4·8}$$

where Ψ, ψ, ϕ and $F_{\lambda\mu}=\partial_\lambda A_\mu-\partial_\mu A_\lambda$ are the wave functions of the isobar, nucleon and pion and the field strength of the electromagnetic field, and

$$O=\begin{cases}1\\ i\gamma_5,\end{cases}\qquad O'=\begin{cases}\gamma_5, & \text{for pseudospinor isobar,}\\ 1, & \text{for spinor isobar.}\end{cases} \tag{4·9}$$

We may reasonably assume that the nucleon is spinor and the pion pseudoscalar[11], but there remains a question whether the isobar is spinor or pseudospinor, so that two possibilities are taken into account in the interactions (4·7) and (4·8).

---

* We employed the same representation with that by Nambu and Yamaguchi.[10]

As for the charge dependence of the first Lagrangian $\mathfrak{L}_1$, we have only to refer to the expression (4·6).

The coupling constant ε in $\mathfrak{L}_2$ must be distinguished between states with the charge $+e$ and 0, i.e.,

$$\varepsilon_P \quad \text{for} \quad \gamma+p \to \mathfrak{N}_1,$$
$$\varepsilon_N \quad \text{for} \quad \gamma+n \to \mathfrak{N}_0.$$

We can derive no relation between ε_P and ε_N from the symmetrical theory. If we assume, however, that the contribution from the pion current overcomes that from the nucleon current in such radiative processes at low energies under consideration, we may adopt a relation:

$$\varepsilon_P \approx -\varepsilon_N, \tag{4·10}$$

just as that between the anomalous magnetic moments of the proton and neutron.

The forms of the interaction Lagrangians (4·1) and (4·2) which are invariant under the Lorentz and gauge transformation are unique within the frame of the canonical formalism.*)

§ 5. Resonance and damping effects

In calculating the matrix elements of pion reactions, there happens sometimes the conservation of energy in an intermediate state:

$$\pi+N \to \mathfrak{N}$$

which leads to a resonance.

In order to avoid the vanishing denominator, we must take account of the damping effect, and for this purpose we have to pick up suitable terms from higher order processes. The Feynman graphs for the pion-nucleon scattering are given by (a), (b), (c) and (d) in fig. 1.

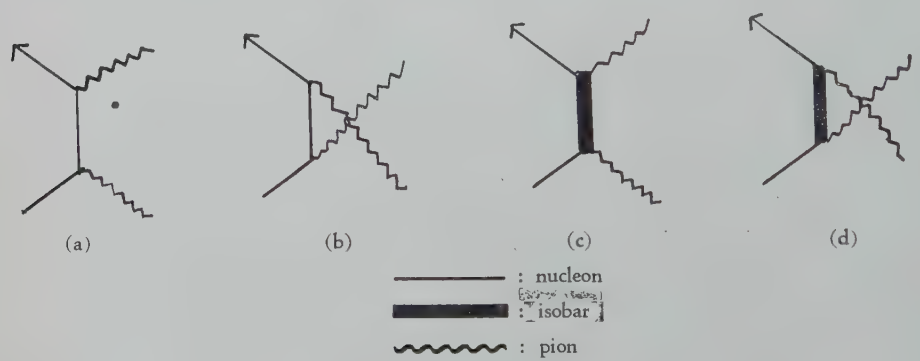

Fig. 1

* The condition of gauge invariance requires further to replace $\partial_\mu\phi$ and $\partial_\mu\phi^*$ in the Lagrangian $\mathfrak{L}_1$ by $(\partial_\mu - ieA_\mu)\phi$ and $(\partial_\mu + ieA_\mu)\phi^*$ respectively. The additional terms, however, do not contribute to the matrix elements of the order we are interested in.

Fig. 1 (c) is the graph that gives rise to the resonance and consequently requires the introduction of the damping. For other graphs we shall neglect such effects arising from higher order processes, because they may be small at low energies in question.

The damping may be introduced, if one replaces the contribution from graph (c) by the sum of contributions from a series of graphs (c^1), (c^2),$\cdots$ in fig. 2.

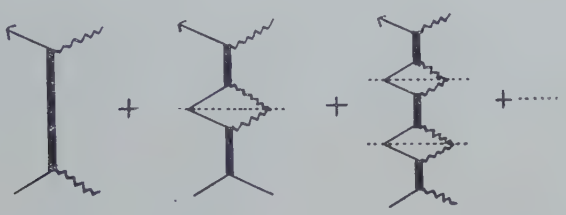

Fig. 2

·····: the line indicating the occurence of the real nucleon and pion.

This procedure seems to provide us the most simple means for our purpose.

The substitution of $(c^1)+(c^2)+\cdots$ into (c) results in the modification of its propagation function $\mathfrak{S}_F$.

The propagation function written in the momentum space is given by

$$\mathfrak{S}_F(p)=\frac{1}{2\pi i}\left(\frac{1}{D(ip)}\right)_{M\to M-i\varepsilon}. \tag{5·1}$$

The above substitution modifies $\mathfrak{S}_F$ as

$$\bar{\mathfrak{S}}_F=\mathfrak{S}_F+\mathfrak{S}_F N\mathfrak{S}_F+\mathfrak{S}_F N\mathfrak{S}_F N\mathfrak{S}_F+\cdots, \tag{5·2}$$

where

$$N_{\lambda\mu}(p)=-\frac{1}{2\mu^2}\left(\frac{G^2}{4\pi}\right)\int(dq)\,q_\lambda q_\mu\, O\left[i\gamma(p+q)-m\right]O\delta\left[(p+q)^2+m^2\right]\delta(q^2+\mu^2), \tag{5·3}$$

which vanishes for $p^2+(m+\mu)^2>0$.

The integration yields

$$N_{\lambda\mu}(p)=-\frac{1}{2\mu^2}\left(\frac{G^2}{4\pi}\right)\left[O(i\gamma p-m)\,O\cdot A_{\lambda\mu}(p)+B_{\lambda\mu}(p)\right], \tag{5·4}$$

where

$$A_{\lambda\mu}(p)=\pi\frac{\varepsilon(p)}{\sqrt{-p^2}}P\cdot Q\left[\delta_{\lambda\mu}\cdot P+\frac{p_\lambda p_\mu}{p^2}(P-Q)\right],$$

$$B_{\lambda\mu}(p)=i\frac{\varepsilon(p)}{\sqrt{-p^2}}Q\left[p_\lambda A_{\mu\rho}\gamma_\rho+p_\mu A_{\lambda\rho}\gamma_\rho+(\gamma p)A_{\lambda\mu}\right],$$

$$\varepsilon(p)=\frac{p_0}{|p_0|},\quad P=\sqrt{\frac{\{p^2+(m+\mu)^2\}\{p^2+(m-\mu)^2\}}{-4p^2}},\quad Q=\sqrt{\frac{(p^2+m^2-\mu^2)^2}{-4p^2}}.$$

The following relations are worth noticing in practical calculations :

P=pion momentum, Q=pion energy

in the center of mass system.

Now the infinite sum (5·2) gives

$$\bar{\mathfrak{S}}_F(p)=\frac{1}{2\pi i}\cdot\frac{1}{D(ip)-(2\pi i)^{-1}N(p)}\,. \tag{5·5}$$

On account of (5·4), we readily see that $\bar{\mathfrak{S}}_F(p)$ can well be approximated at low energies by replacing the expression p^2+M^2 which appears in the denominator of $\mathfrak{S}_F(p)$ by

$$(1-A_1-B_1)^2p^2+(M+mO^2\cdot A_1)^2, \tag{5·6}$$

provided that the coupling constant $G^2/4\pi$ is not so large*).

The quantities A_1 and B_1 in the expression (5·6) are defined by

$$A_1=\frac{i}{4\mu^2}\left(\frac{G^2}{4\pi}\right)\frac{\varepsilon(p)}{\sqrt{-p^2}}P^2Q\,,\quad B_1=\frac{i}{4\mu^2}\left(\frac{G^2}{4\pi}\right)\frac{P^2Q^2}{-p^2}\,. \tag{5·7}$$

Part II. Pion-Proton Scattering

§ 6. Formulation

The Lagrangian expressing the interaction among pion, nucleon and electromagnetic fields is given by

$$\begin{aligned}L_{int.}=&-if\bar{\psi}\gamma_5\tau_j\psi\cdot\phi_j+ie\bar{\psi}\tau_P\gamma_\lambda\psi\cdot A_\lambda\\&+eA_\lambda\left(\phi_1\frac{\partial\phi_2}{\partial x_\lambda}-\frac{\partial\phi_1}{\partial x_\lambda}\phi_2\right)-\frac{1}{2}e^2A_\lambda^2(\phi_1^2+\phi_2^2)\\&-i\frac{g}{\mu}\bar{\psi}\gamma_5\gamma_\lambda\tau_j\psi\cdot\frac{\partial\phi_j}{\partial x_\lambda}+\frac{g}{\mu}\bar{\psi}\gamma_5\gamma_\lambda[\tau_j\tau_I]\psi\cdot A_\lambda\phi_j\,,\end{aligned} \tag{6·1}$$

to which we must further supplement the Lagrangians $\mathfrak{L}_1$ and $\mathfrak{L}_2$. Then the transition matrix R corresponding to the pion-proton scattering can be written as

$$R=c_aR_a+c_bR_b+c_cR_c+c_dR_d\,, \tag{6·2}$$

where (cf. fig. 1)

$$R_a=-\frac{i}{2\sqrt{2}\,(2\pi)^2}f^2\bar{u}(F)\gamma_5\frac{i\gamma(I+q_i)-m}{(I+q_i)^2+m^2}\gamma_5u(I),$$

$$R_b=-\frac{i}{2\sqrt{2}\,(2\pi)^2}f^2\bar{u}(F)\gamma_5\frac{i\gamma(I-q_f)-m}{(I-q_f)^2+m^2}\gamma_5u(I),$$

$$R_c=\frac{i}{12(2\pi)^2}\left(\frac{G}{\mu}\right)^2\bar{u}(F)O(q_f)_\lambda\bar{\mathfrak{S}}_F(I+q_i)_{\lambda\rho}(q_i)_\rho Ou(I),$$

* Rigorously speaking, this condition is very severe in the case of spinor isobar.

$$R_d=\frac{i}{12(2\pi)^2}\left(\frac{G}{\mu}\right)^2\bar{u}(F)O(q_i)_\lambda \mathfrak{S}_F(I-q_f)_{\lambda\rho}(q_f)_\rho Ou(I), \tag{6·3}$$

where I, F, q_i and q_f denote the four momenta of the initial and final nucleons and of the pions respectively, and for brevity only the case of pseudoscalar coupling is illustrated in the above expression. The coefficients c's are tabulated in Table I.

Table I.*)

Scattering Mode	c_a	c_b	c_c	c_d
$\pi^+ + p \to p + \pi^+$	0	$\sqrt{2}$	3	1
$\pi^- + p \to p + \pi^-$	$\sqrt{2}$	0	1	3
$\pi^- + p \to n + \pi^0$	-1	1	$\sqrt{2}$	$-\sqrt{2}$

Let R^+, R^- and R^0 be the transition matrices corresponding to the above three modes of scattering, then in the symmetrical theory holds the following formula:

$$R^+ - R^- = \sqrt{2}\, R^0. \tag{6·4}$$

For practical calculations, it is useful to note that the Dirac equation is of help to reduce the γ-dependence of the transition matrix into the linear combination of two fundamental forms:[12]

$$R = aU_1 + bU_q, \tag{6·5}$$

with

$$U_1=\bar{u}(F)u(I), \quad U_q=\bar{u}(F)\frac{(i\gamma q_i)}{m}u(I).$$

The propagation function $\mathfrak{S}_F(p)$ employed in this section differs from the one in the previous section by a factor $2\pi i$, and is given by

$$\mathfrak{S}_F(p)_{\lambda\rho}=\frac{1}{p^2+M^2}\Big[\delta_{\lambda\rho}(i\gamma p-M)+\frac{2}{3M^2}p_\lambda(i\gamma p)p_\rho-\frac{4}{3M}p_\lambda p_\rho-\frac{i}{3M}\{p_\lambda(i\gamma p)\gamma_\rho+\gamma_\lambda(i\gamma p)p_\rho\}$$
$$-\frac{i}{M^2}\left\{\frac{2}{3}p^2+M^2\right\}\{\gamma_\lambda p_\rho+p_\lambda\gamma_\rho+i\gamma_\lambda(i\gamma p+M)\gamma_\rho\}\Big].$$

§ 7. Results of calculations

In this section, we shall first decide whether the isobar is spinor or pseudospinor. Since the contribution from graph (c) is the largest at energies near resonance, we may make a rough estimate of the total cross section for $\pi^+ - p$ scattering only by graph (c). The denominator of the propagation function

$$(1-A_1-B_1)^2p^2+(M+mO^2\cdot A_1)^2$$
$$\approx(p^2+M^2)-2p^2(A_1+B_1)+2mMO^2\cdot A_1 \tag{7·1}$$

reduces just at the resonance energy to

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* We have chosen the isotopic spin matrix τ_3 as to satisfy

$$\tau_3 p=p, \quad \tau_3 n=-n.$$

$$2M^2(A_1+B_1)+2mMO^2\cdot A_1\,. \qquad (7\cdot 2)$$

The quantities A_1 and B_1 are proportional to G^2, so that the matrix element just at the resonance energy is independent of the magnitude of the coupling constant G. Hence we shall study the dependence of the total cross section upon the excitation energy of the isobar. The pseudospinor isobar gives a reasonable magnitude of σ^+, as shown in fig. 3, whereas the spinor isobar gives too small σ^+ to account for observed cross sections. Hence we shall hereafter investigate only the case of pseudospinor isobar.

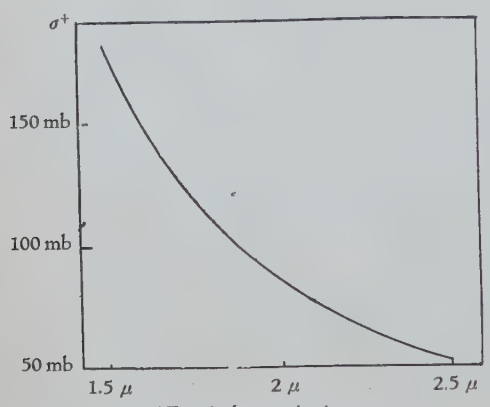


Fig. 3. The total cross section σ^+ at just the resonance energy calculated from the graph (c) *vs.* the isobar excitation energy.

Even in the case of pseudospinor isobar the total cross section is less than the experimental one. This fact indicates that states other than $I=J=3/2$ appreciably contribute to cross sections at energies near resonance.[13]

A. *Case of Pseudovector Coupling*

Next we shall study the case in which only the pseudovector coupling is taken into account between pion and nucleon.

The results are shown in fig. 4. The absolute values of cross sections are smaller than those observed by a factor 2 at energies near resonance and much smaller at low energies.

This is due to the oversimplification of the model and also to the inadequacy of the pure pseudovector coupling. The steep drop of σ^+ over the resonance energy results from the destructive interference between the contributions of the graph (c) and others. The tendency of the excitation functions and the ratio $\sigma^+:\sigma^-:\sigma^0$ are consistent with experiments as it is expected from the beginning. The calculated angular distributions, however, are markedly contrasted with those observed, in which the backward scattering is predominant.[14] The narrow width is due to the choice of small magnitude of the coupling constant, i.e., $G^2/4\pi=0.1$.

These defects indicate the necessity of the inclusion of the pseudoscalar coupling in order to enhance the S scattering of pions.

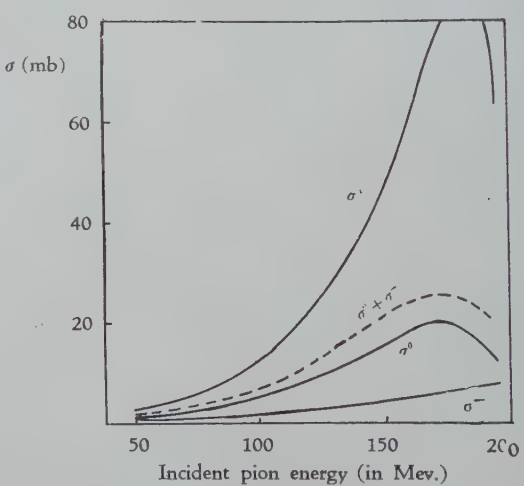


Fig. 4. The excitation functions of the pion-proton scattering.
$\Delta E=2\mu$,
$G^2/4\pi=0.1$,
$g^2/4\pi=(0.4)^2=0.16$.

Since the coupling of pion S wave with nucleon increases by taking also the pseudoscalar coupling into account, the total cross sections will go up at low energies and the angular distributions will approach to the experimental ones due to the interference between S and P waves.

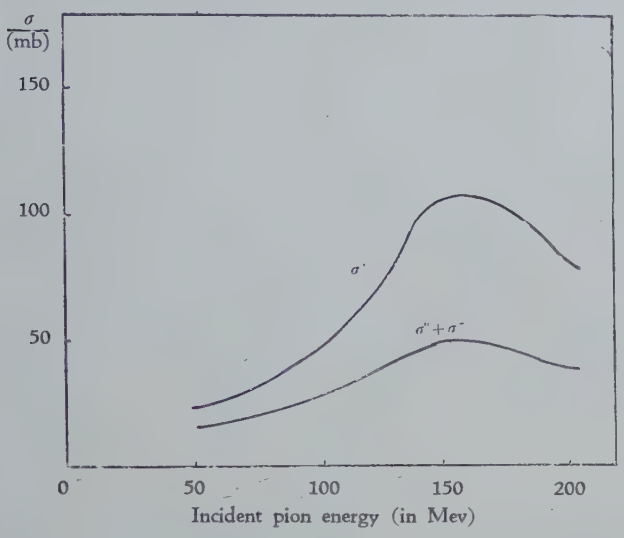


Fig. 5. The excitation functions of the pion-proton scattering.
$\Delta E=2\mu$,
$G^2/4\pi=0.2$,
$f^2/4\pi=1.5$.

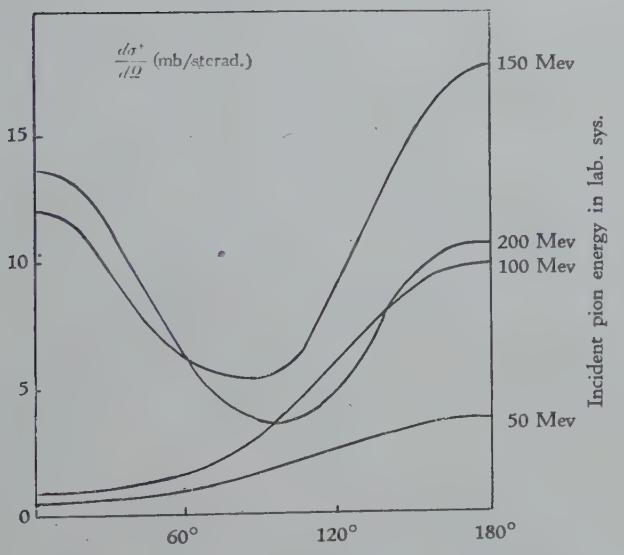


Fig. 6. The angular distributions of the scattering
$\pi^+ + p \to p + \pi^+$
in the centre of mass system.

B. *Case of Pseudoscalar Coupling*

To see the rôle of the pseudoscalar coupling, we shall show the results of calculation with the pure pseudoscalar coupling in fig. 5 and fig. 6.

All defects of the pseudovector coupling are remedied. The ratio, however, becomes worse and the magnitude of the coupling constant $f^2/4\pi=1.5$ is too small to account for the photo-pion production as will be seen later.

Thus we may conclude that the inclusion of both pseudoscalar and pseudovector couplings is necessary and indeed it gives a better agreement with experiments, which will be published elsewhere.

Part III. Photo-Pion Production

§ 8. Calculation of the photo-pion cross sections

In this section, we calculate the cross sections of the photo-pion production according to the method adopted in Part II.

The Feynman graphs for the photo-pion production are given in fig. 7.

Let the matrix elements corresponding to the above graphs

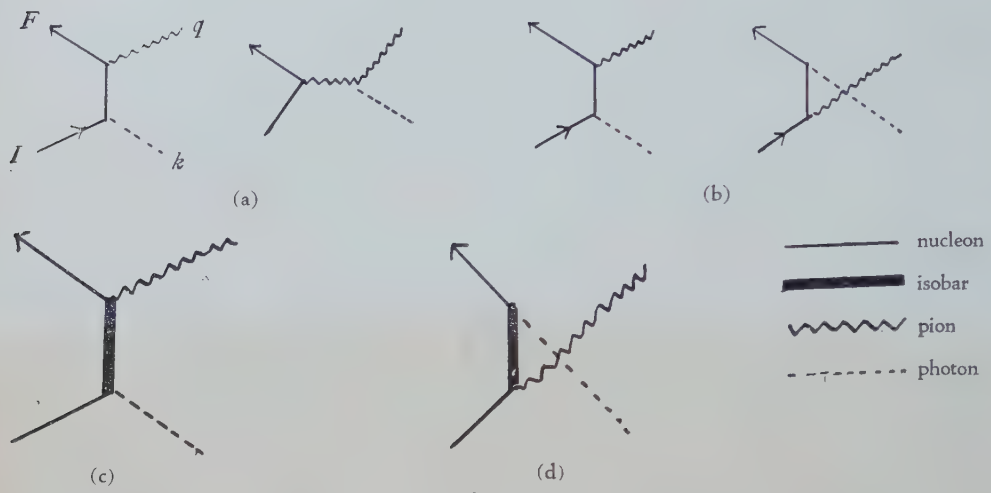


Fig. 7

be R_a, R_b, R_c and R_d, then R's are given by

$$R_a=-\frac{eF}{(4\pi)^2}\left[-\frac{1}{a}U_m+\frac{b}{a-b}U_c\right],$$

$$R_b=-\frac{eF}{(4\pi)^2}\left[\frac{a-b}{ab}U_m-U_c\right],$$

$$R_c=-\frac{\epsilon_P G}{(4\pi)^2}\cdot\frac{1}{\sqrt{3}}\left(\frac{m}{\mu}\right)\frac{i}{D+iE}\left[-\left(\frac{M}{m}+1\right)bU_A^{(2)}\right.$$
$$+2a\left\{\left(\frac{M}{m}+1\right)\left(\frac{3}{2}-\frac{4m^2}{3M^2}\right)+\frac{\mu^2}{6M^2}-\frac{m^2}{2M^2}a\left(3\frac{M}{m}+\frac{7}{3}\right)\right\}U_A^{(1)}$$
$$\left.+\frac{ab}{2}U_c+\left\{\frac{\mu^2}{m^2}\left(1+\frac{m}{3M}-\frac{m^2}{3M^2}\right)-\frac{a}{2}\left(2+\frac{\mu^2}{M^2}-\frac{m}{3M}-\frac{4m^2}{3M^2}\right)+\frac{m^2}{2M^2}a^2+\frac{b}{2}\right\}U_m\right],$$

$$R_d=-\frac{\epsilon_N G}{(4\pi)^2}\frac{1}{\sqrt{3}}\left(\frac{m}{\mu}\right)\frac{i}{b+(M^2/m^2)-1}\left[\left(\frac{M}{m}+1\right)aU_A^{(1)}\right.$$
$$-2b\left\{\left(\frac{M}{m}+1\right)\left(\frac{3}{2}-\frac{4m^2}{3M^2}\right)+\frac{\mu^2}{6M^2}+\frac{m^2}{2M^2}b\left(3\frac{M}{m}+\frac{7}{3}\right)\right\}U_A^{(2)}$$
$$\left.+\frac{ab}{2}U_c+\left\{\frac{\mu^2}{m^2}\left(1+\frac{m}{3M}-\frac{m^2}{3M^2}\right)+\frac{b}{2}\left(2+\frac{\mu^2}{M^2}-\frac{m}{3M}-\frac{4m^2}{3M^2}\right)+\frac{m^2}{2M^2}b^2-\frac{a}{2}\right\}U_m\right], \tag{8·1}$$

where

$$F=f+\frac{2m}{\mu}g,^{*)}$$

* It must be remembered that the equivalence theorem holds in the photo-pion production.

$$a=-\frac{2(Ik)}{m^2}, \quad b=-\frac{2(Fk)}{m^2},$$

$$D+iE=(1/m^2)[(1-A_1-B_1)^2(I+k)^2+(M+mA_1)^2],$$

$$U_e=\bar{u}(F)\left\{\frac{iF_\mu}{(Fk)}-\frac{iI_\mu}{(Ik)}\right\}i\gamma_5 u(I)\cdot A_\mu(k): \text{ nucleon current,}$$

$$\left.\begin{aligned} U_m&=\bar{u}(F)i\gamma_5\frac{\sigma_{\mu\nu}k_\nu}{m^2}u(I)\cdot A_\mu(k)\\ U_A^{(1)}&=-\bar{u}(F)i\gamma_5\frac{i\gamma(I+k)-m}{(I+k)^2+m^2}\cdot\frac{\sigma_{\mu\nu}k_\nu}{2m}u(I)\cdot A_\mu(k)\\ U_A^{(2)}&=-\bar{u}(F)\frac{\sigma_{\mu\nu}k_\nu}{2m}\cdot\frac{i\gamma(F-k)-m}{(F-k)^2+m^2}\cdot i\gamma_5 u(I)\cdot A_\mu(k) \end{aligned}\right\}\text{ magnetic interaction.} \qquad (8\cdot2)$$

It is well known that matrix elements of the photo-pion production can always be expressed as the linear combinations of the above four elementary forms[15] (8·2).

Then the transition matrix of the photo-pion production is written as

$$R=c_aR_a+c_bR_b+c_cR_c+c_dR_d$$

where the coefficients c's, being characteristic numbers for each mode of the production, are given in Table II.

Table II*)

Production Mode	c_a	c_b	c_c	c_d
$\gamma+p\to n+\pi^+$	1	0	1	1
$\gamma+p\to p+\pi^0$	0	1	$\sqrt{2}$	$\sqrt{2}$

The results of the calculation are given in fig. 8 and fig. 9.

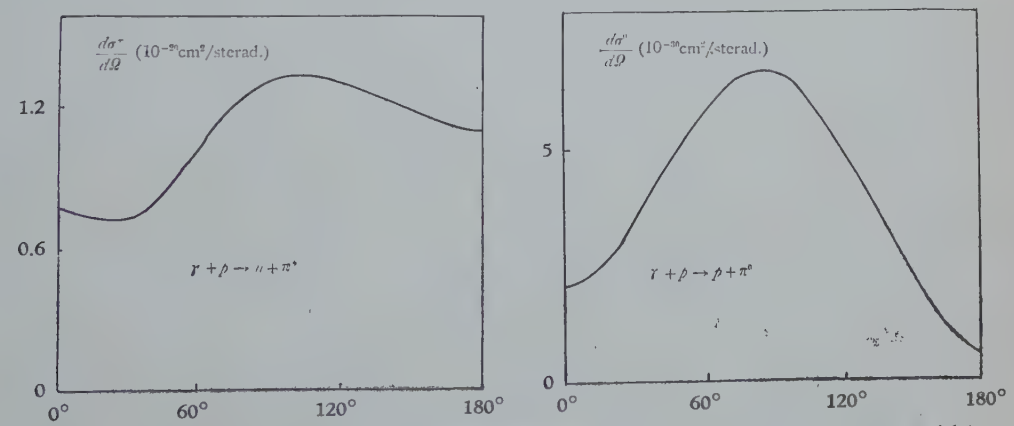
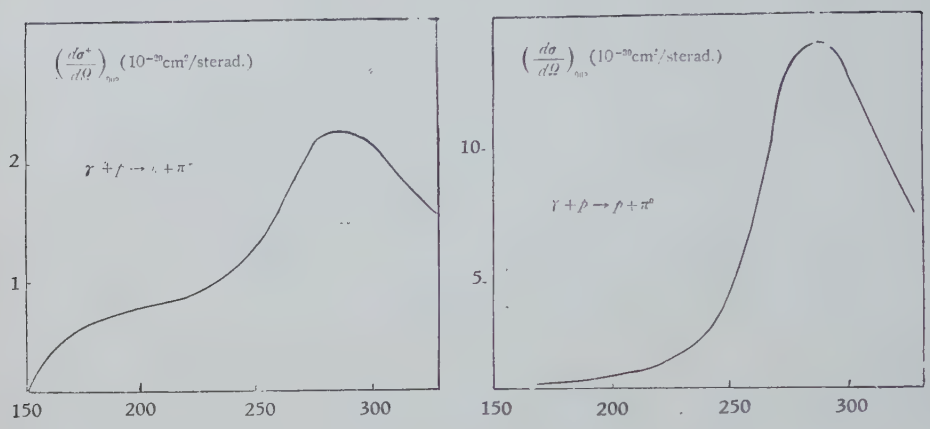


Fig. 8. Angular distributions in the centre of mass system at 255 Mev. incident photon energy (in lab.)

* We let $\varepsilon_P=-\varepsilon_N$ for simplicity. Cf. (4·10).



Parameters: $\Delta E = 1.75\,\mu$, $F^2/4\pi = \left(0.4 \times \frac{2m}{\mu}\right)^2$, $G^2/4\pi = 0.1$,

$\varepsilon_P = -\varepsilon_N$, $\varepsilon_P G/eF = 1.2(\mu/2m)$.

Fig. 9. The excitation functions at 90°.

§ 9. Comparison with other theories

The photo-pion production has so far been investigated by many authors[16]. The experimental results indicate that the electric dipole and magnetic dipole transitions give the same order of contributions to the positive pion production and the non-static effect of the magnetic moment of nucleon takes a main part in neutral pion production.

Our result shows the excitation functions more or less similar to those of Brueckner and Case,* and the tendency seems to be consistent with experiments.

The theoretical angular distribution of the positive pions is in fair agreement with experiments,[17] since the interference of the electric dipole and magnetic dipole transitions is correctly taken into account by choosing the sign of $\varepsilon_P G$ equal to that of eF.

The theoretical angular distribution of neutral pions is consistent with the experimental result of Silverman and Stearns[18] at incident photon energies of 250 ~ 300 Mev.

$$\left(\frac{d\sigma^0}{d\Omega}\right)_{76°} \Big/ \left(\frac{d\sigma^0}{d\Omega}\right)_{112°} = 1.1 \pm 0.2$$

in the center of mass system, but not with the preliminary result of Panofsky, Steinberger and Steller,[19] in which produced neutral pions are peaked in the forward direction.

As for this point, the higher order calculation yields better agreement.[20] Next, we shall compare the contribution from the isobar with that from an orthodox higher order calculation.

For this purpose, it is convenient to express the total matrix element but the lowest order as a linear combination of the four fundamental forms, U_m, U_c, $U_A^{(1)}$ and $U_A^{(2)}$, i.e.,

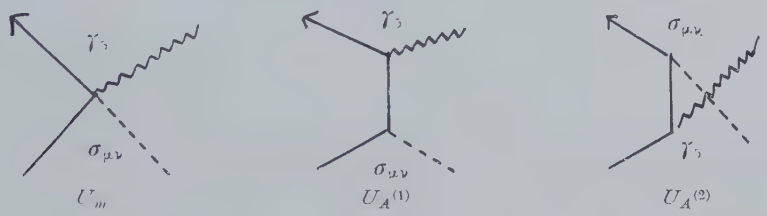
* Notice that ours are the excitation functions at 90°, while those of Brueckner and Case are the total.

$$G_m U_m + G_c U_c + G_A^{(1)} U_A^{(1)} + G_A^{(2)} U_A^{(2)},$$

where the coefficients G's, being functions of angle and energy, are generally complex numbers.

Since the contribution from a current type interaction $G_c U_c$ is negligibly small, our discussions are mainly devoted to the magnetic type interactions.

The qualitative behaviour of the angular distribution is governed according as which of the three types, U_m, $U_A^{(1)}$ and $U_A^{(2)}$, contributes mainly to the cross section. (Cf. fig. 10)



U_m $U_A^{(1)}$ $U_A^{(2)}$

Fig. 10

We shall then discuss the angular distribution for the neutral pion production in which the higher order contributions are remarkable.

(1) In the higher order calculation, the term $G_m U_m$ becomes overwhelmingly large, and furthermore G_m is nearly independent of angle, so that produced pions are pronounced in the forward direction.

(2) The phenomenological introduction of a Pauli term[21] to represent the effect of the anomalous magnetic moment of the proton in the pseudoscalar coupling theory corresponds to let $G_m = G_c = 0$, $G_A^{(1)} = G_A^{(2)} = \mu_P$ (const.). Thus produced pions are peaked in the backward direction. In the case of pseudovector coupling, the inequivalent term changes G_m by a constant factor as to increase the differential cross section in the forward direction.

(3) Although the contributions from $G_m U_m$ cannot be neglected in our present calculation, it is essentially important that $G_A^{(1)}$ and $G_A^{(2)}$ occur with opposite signs so as to make $G_A^{(1)} + G_A^{(2)}$ decrease with increasing angle, and consequently the differential cross section becomes maximum near 90°. That $G_A^{(1)}$ and $G_A^{(2)}$ have opposite signs leads to the superiority of non-static effects* just as in the case of the higher order calculation.

Part IV. Discussions

§ 10. Discussions of the results

To all theories that admit the existence of the nucleon isobar, the main features of their results are common. For instance, the charge ratio 9 : 1 : 2 (Cf. § 2) and the resonance like behaviour of excitation functions are the immediate consequences.[22]

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* Remember that $G_A^{(1)}$ and $G_A^{(2)}$ have the same value if only the static magnetic moment is considered.

We shall, therefore, fix our attention upon detailed points of the results. In order to interpret the large total cross sections of the pion-proton scattering, we are compelled to recognize the importance of intermediate states other than $I=J=3/2$.

The observed angular distributions also indicate a large contribution from the S state, and the coupling of a nucleon to the pion S wave mainly comes from the pseudoscalar coupling in our theory.

In the strong coupling theory, however, the pion field is separated into bound and unbound parts, and subjected to the following three interactions

$$N N \pi_f, \quad N \mathfrak{N} \pi_f, \quad \mathfrak{N} \mathfrak{N} \pi_f, \quad (\pi_f: \text{ unbound pion}) \tag{10·1}$$

the first and the last ones are prohibited in the lowest order in the strong coupling theory*).

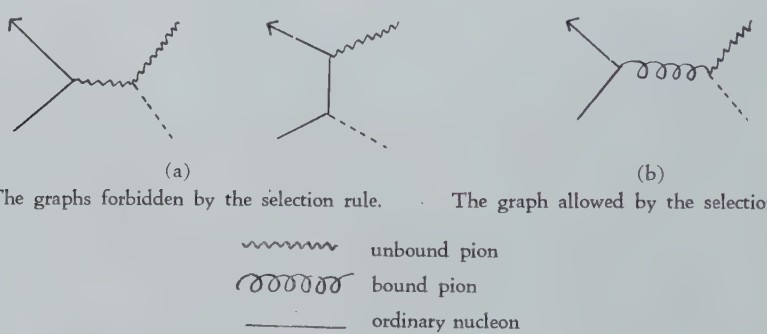
Thus the theory fails to account for the S state interaction, i.e., the graphs (a) and (b) in fig. 1 are forbidden in this theory.

Next we shall proceed to the discussions of the photo-pion production. The ratio σ^+/σ^0 is equal to $1/2$ if only the contribution from the resonant process was considered, (Cf. Table II) while experiments show

$$\left(\frac{d\sigma^+}{d\Omega}\right)_{90^\circ} \Big/ \left(\frac{d\sigma^0}{d\Omega}\right)_{90^\circ} \sim 1 \quad \text{at 300 Mev.}^{24)} \tag{10·2}$$

To remedy this discrepancy we have to increase the cross section of the positive pion production, which is done in our theory by including the matrix elements of the lowest order perturbation theory, thereby remembering the near cancellation of the matrix elements of the neutral pion production.

In the strong coupling theory, the processes expressed by the graphs (a) in fig. 11 are forbidden by the selection rule mentioned above and we have to supplement the ratio only by the process (b) which, however, seems insufficient to improve the situation.



(a) The graphs forbidden by the selection rule.

(b) The graph allowed by the selection rule.

Fig. 11

* This selection rule was pointed out by H. Miyazawa,[23] i.e.,

$$\Delta J = \pm 1.$$

§ 11. Remarks on the nucleon isobars

In this last section, the concept of the nucleon isobar is examined. First, the possibility of explaining the nucleon isobar in terms of the weak coupling theory is considered.

The most interesting processes in the pion-proton scattering are such that the energy is conserved in intermediate states as illustrated in fig. 12.

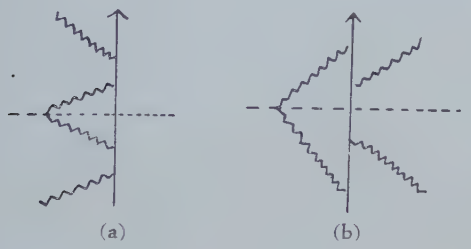
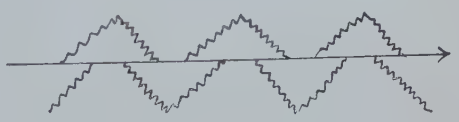


Fig. 12

These processes have intimate correspondence to the nucleon isobars in some sense.

The type (a) is the scattering through a state $I=J=1/2$, and the type (b) involves both $I, J=1/2$ and $3/2$.

Especially in the π^+-p scattering appears only a state with $I=3/2$. The endless repetitions of these diagrams may yield, in the sense of the ladder approximation, nucleon isobars as a possible bound state. (Cf. fig. 13)


The repetition of the graph (b) in fig. 12.
Fig. 13

For instance, the isobar states with $I=J=1/2$ are furnished as the poles of the propagation function $S_F'(p)$. To our regret, however, the method to deal with the metastable states is as yet not known in the theory of bound states.

Next, discussions are made on the validity of the present approximation in which the isobar is regarded as if it were an elementary particle. The error to substitute the complex system composed of a nucleon and a pion by a point particle is due mainly to the neglect of its structure. Mathematically speaking, the local interaction $\mathfrak{N}N\pi$ in our theory can be regarded as the first term of the expansion of the real non-local interaction with respect to the parameter expressing the structure of the isobar.

Let the dimension of the isobar and the wave length of the scattered pion be d and λ respectively, then the condition for our approximation to hold will be

$$\lambda \gg d. \tag{11·1}$$

In our case, however, d is considered to be of the order of $1/\mu \sim 1/2\mu$, so that the condition (11·1) is hardly be satisfied at energies in question, and we are better to interpret the local interaction $\mathfrak{N}N\pi$ as a suitable average of the true interaction in some energy region. If the isobar were really elementary as has been suggested by Pais in his theory of V-particles,[25] however, the above situation will be changed completely.

On the existence of the nucleon isobar, we know yet nothing conclusive, but it does not seriously contradict to experiments. In reality, the lifetime of the isobar seems to be too short ($\hbar/\Gamma \sim 10^{-23}$ sec) to call it a "level".

From the phase shift analysis of a recent experiment on the angular distributions of the pion-proton scattering at 110 and 135 Mev., it is known that the phase shift of the wave with $I=3/2$, $J=3/2$ ($p_{3/2}$) is not so large as to be expected from the existence of a resonance level, i.e., it does not exceed 40° even at 135 Mev.

From the relation[26]

$$\tan\delta = \Gamma(E)/2(E_r - E), \qquad (\delta: \text{phase shift}) \qquad (11\cdot2)^{*)}$$

we see that the level width $\Gamma(E_r)$ just at the resonance energy is at most 70 Mev. in contrast to the observed excitation function.

An experiment on the angular distribution just at the resonance energy will facilitate to judge the existence of the nucleon isobar.

Finally we may conclude that the nucleon isobar, if really existed, will not necessarily lead to the superiority of the strong coupling theory to other approximations, but it can also be criticized as the possible improvement of the interaction model between pion and nucleon fields.

The authors are grateful to Prof. Y. Nambu, Prof. S. Hayakawa, Mr. Y. Yamaguchi, and Mr. H. Miyazawa for their helpful discussions and criticism.

References

1) Rarita and Schwinger, Phys. Rev. **6**) (1941), 61.
2) Steinberger, Panofsky and Steller, Phys. Rev. **78** (1950), 802.
Steinberger and Cook, Phys. Rev. **8**) (1950), 291.
3) M. F. Kaplon, Phys. Rev. **8**3 (1951), 206.
Aidzu, Fujimoto and Fukuda, Prog. Theor. Phys. **6** (1951), 193.
4) Fujimoto and Miyazawa, Prog. Theor. Phys. **5** (1950), 1052.
Brueckner and Case, Phys. Rev. **8**3 (1951), 1141.
5) Anderson et al., Phys. Rev. **85** (1952), 936.
6) K. A. Brueckner, Phys. Rev. **86** (1952), 106.
7) Anderson et al., Phys. Rev. **86** (1952), 793.
8) Watson and Brueckner, Phys. Rev. **8**3 (1951), 1.
9) Pauli and Dancoff, Phys. Rev. **6**2 (1942), 85.
10) Nambu and Yamaguchi, Prog. Theor. Phys. **6** (1951), 1000.
11) Yang and Tiomno, Phys. Rev. **79** (1950), 495.
12) Nakano and Nishijima, Prog. Theor. Phys. **8** (1952), 53.
13) See ref. (5).
14) See ref. (7).
15) Koba, Kotani and Nakai, Prog. Theor. Phys. **6** (1951), 849.
S. Minami, Prog. Theor. Phys. **7** (1952), 69.
16) See ref. (3), (4) and (15). Also see Brueckner and Watson, Phys. Rev. **86** (1952), 923.
17) Steinberger and Bishop, Phys. Rev. **86** (1952), 171.
18) Silverman and Stearns, Phys. Rev. **8**3 (1951), 853.
19) Panofsky, Steinberger and Steller, Phys. Rev. **86** (1952), 180.
20) See ref. (15).
21) See ref. (3).
22) See ref. (6). Also see G. Wentzel, Phys. Rev. **86** (1952), 437.
23) Matsuyama and Miyazawa, Prog. Theor. Phys. **8** (1952), 140.
24) See ref. (18).
25) A. Pais, Phys. Rev. **86** (1952), 663.
26) Feshbach, Peaslee and Weisskopf, Phys. Rev. **71** (1947), 145.

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* A rough estimate is made by assuming $\Gamma(E) \propto (\text{pion momentum})^3$.

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Phenomenological Explanation of Magnetic Moments of Nucleons in Terms of the Excited States of Nucleons

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The anomalous magnetic moment of nucleons are explained phenomenologically by inclusion of the virtual transition to excited state of $\sigma=3/2$ and $\tau=3/2$ accompanied by one meson emission in addition to the usual virtual transitions of nucleon states accompanied by meson emissions. The inclusion of excited state of $\sigma=3/2$ and $\tau=3/2$ is definitely essential and the inclusion of other excited states of $\sigma=3/2$ and $\tau=1/2$ or $\sigma=1/2$ and $\tau=3/2$ is of no effect. Six interesting conclusions are obtained and given in the first section. The other sections are concerned with the derivations and discussions of these conclusions.

§ 1. Introduction and summary

The anomalous magnetic moments of nucleons are well explained qualitatively in terms of the meson clouds around the nucleons. However, the quantitative calculations show us that the meson theory gives uncorrected values of the anomalous magnetic moments of nucleons to the second order perturbation calculations[1]. This reveals that the second order perturbations are quite unsatisfactory in meson theory. According to the considerations that the fourth order contributions might be the same order of magnitude as the second order ones owing to the appearing of the factor γ_5 in pseudoscalar meson theory, the fourth order calculations were made by Nakabayasi and Sato[2] using pseudoscalar coupling in pseudoscalar meson theory, in which the renormalization techniques are successful. These calculations show that the radiative corrections are clearly in direction to remove the discrepancy existing in the lowest order and it is possible to give the correct moments both for neutron and proton by appropriately adjusting coupling constants.

It is here to be noted that the above calculations are only concerned with the anomalous parts of the magnetic moments of nucleons and do not take into account the decrease of the normal part of the magnetic moment of proton originating from the umklapping of τ-spin and ordinary spin due to virtual π-meson emission. In meson theory the perturbation are not always small and in such a case the probability that the system is in its unperturbed state cannot be put equal to one but must be reduced by the amount that the syetem is in perturbed states. Furthermore one cannot readily say whether the next higher order corrections are really small or not.

In order to investigate these problems quantitatively we must have recourse to the intermediate-coupling-theoretical calculations. Concerning the magnetic moments of nucleons,

the state of a nucleon, which is surrounded by the meson clouds around it, can be expanded in terms of a state in which the nucleon is bare and in its normal state and states in which several π-mesons are present besides a bare nucleon. The expansion coefficient of the state of no meson present, which is an unperturbed state, is certainly less than one, thus taking into account the decrease of the normal part of magnetic moment of proton caused by the meson clouds around it. In the above expansion we suppose that the expansion coefficient of the state of two mesons present is never negligible compared with the one of one meson present. It must here be pointed out that, when the meson clouds consist of two mesons, one of the two mesons may possibly be coupled so strongly with the nucleon in its normal state that the nucleon may be transformed into some excited state of a nucleon, just as in the case of meson-nucleon scattering, where the nucleon may be excited to its excited state accompanied by π-meson absorption[3]. Therefore a virtual transition may occur in which a nucleon emits one meson and undergoes a transformation into its excited state as frequently as the virtual two π-meson-emission process if the excited state of a nucleon is really so intimately connected with its ground state as is indicated by the scattering experiment. If this is the case, we must add an additional term which represents a virtual state in which an nucleon in its excited state and one meson is present, in the above expansion of a free nucleon state interacting with its surrounding meson field. We may consider the introduction of this new ket vector as the all-inclusive estimation of higher order corrections or as well as a modification of the present theory by introducing another new freedom of a nucleon which prescribes whether the nucleon is in its ground state or in its excited state.

It is the purpose of this investigation to show by phenomenological calculations how well the anomalous magnetic moments are explained by addition of a term which represents a virtual transition to an excited state accompanied by one meson emission in the expansion of a free nucleon state in terms of states of a bare nucleon and some mesons preseht. For simplicity and in order to obtain main features of the above idea, we shall consider only charged meson theory. Only it is here to be remarked that the inclusion of neutral mesons is in general not favourable to the anomalous magnetic moments of nucleons according to the present investigation, which is contrary to the results of Nakabayasi and Sato[2], who conclude that the higher order corrections are really in the direction to remove the discrepancy existing in the lowest order and further the inclusion of neutral mesons is decisively effective. It seems to the author that the above discrepancy arises from the crudeness of the present investigations and more detailed analysis may rather miss the way on account of the rough treatment of the present paper. In order to gain general features correctly from the present rough phenomenological investigations, we do not go into further details. As an another important assumption, we assumed that the virtually emitted mesons have all angular momentum $\pm\hbar$ with regards to the direction of nucleon spin, which is a reasonable assumption theoretically, because pseudoscalar mesons interact with nucleons only in p-state, which is even an exact situation in the weak coupling limit. Thus our considerations are only concerned with virtual meson emissions accompanied by the umklapping of ordinary spin and isotopic spin at the same time.

The present author have investigated throughout many other possibilities and it turned out that the main conclusions itemized below are not modified. However details are not given below because they might miss the way owing to the crude treatments. For example that the inclusion of neutral mesons does not favor is excluded, because it is contradictory to the conclusions of the exact calculations of Nakabayasi and Sato[2]. The main conclusions are summarized in the following:

i) If we are limited only to virtual states of one meson present, we can never attain satisfactory agreement with experiments.

ii) The inclusion of virtual states of two mesons present improves the situation very much and the empirical values can be reproduced by adjusting parameters. However above adjustment of parameters cannot be considered to be completely satisfactory on physical backgrounds.

iii) The inclusions of virtual states of three or more mesons present do not show the inclination to improve the situation step by step. Therefore it is unnecessary to include the virtual states of three or more mesons present in order to fit the anomalous magnetic moments of nucleons.

iv) Above considerations all take into account the decrease of the normal part of magnetic moment of proton caused by the meson clouds around it. The neglect of these modifications has very large effect on the values of magnetic moments and the complete agreement can be attained simply by adding the virtual states of two mesons present if we neglect the above considerations.

v) By the inclusion of virtual transition to excited state of $\sigma=3/2$ and $\tau=3/2$, the situation is further improved and the completely satisfactory adjustments of parameters are possible, where the inclusion of above excited state is essential, therefore the usual virtual transitions accompanied by one or two mesons emission may be modified quite arbitrarily and can be made vanished without affecting the situations at all.

vi) The inclusion of other excited states, namely, of $\sigma=3/2$ and $\tau=1/2$ or of $\sigma=1/2$ and $\tau=3/2$, does not improve the situation at all. Therefore the inclusion of an excited state of $\sigma=3/2$ and $\tau=3/2$ is definitely required.

In the following sections, the above six conclusions are derived successively. In the final section are given the discussions concerning the above introduced excited state of nucleons.

§ 2. One meson emission

If we are limited only to virtual states of one meson present, we have only to include the following two virtual states symbolized below in the expansion of a nucleon state interacting with its surrounding meson field in terms of various virtual states. According to the assumption made in the preceding section which restricts considerations only to charged theory and only to π-meson emission having angular momentum $\pm\hbar$ with regard to the direction of nucleon spin, the only possible virtual states are

$$\begin{aligned} &\text{for Proton;} \quad P(+1/2) \text{ and } N(-1/2)+\pi^{+}(+1), \\ &\text{for Neutron;} \quad N(+1/2) \text{ and } P(-1/2)+\pi^{-}(+1) \end{aligned} \tag{1}$$

where the figures in the parentheses represent the values of angular momenta in the directions of nucleon spins. Let a be the fraction of time in which one meson is emitted. Then the fraction of time in which a nucleon is in its normal state is $1-a$. The magnetic moments of a proton and a neutron are given by the following formulae in units of nuclear magneton :

$$\begin{aligned} \mu_P &= 1-a+a(M/m^*), \\ \mu_N &= -a-a(M/m^*), \end{aligned} \tag{2}$$

where M is nucleon mass and m^* is certain mean value of the relativistic mass of emitted meson and is certainly larger than the rest mass of π-meson owing to relativistic increase of meson inertia, which is definitely required in order to explain the relatively small meson current contributions to magnetic moments compared with the nucleon contributions in the exact calculations[2]. In order to gain the agreement with empirical values $\mu_P=2.7896$ and $\mu_N=-1.9103$, we first add and subtract the two equations (2) :

$$\begin{aligned} \mu_P+\mu_N &= 1-2a=0.8793, \\ \mu_P-\mu_N &= 1+2a(M/m^*)=4.6999. \end{aligned} \tag{3}$$

Thus the values obtained from (3) are

$$a=0.0604, \qquad m^*=60\mathrm{m}_e, \tag{4}$$

where m_e is electron mass. Above value of m^* is too small compared with the rest mass of π-meson. *It is shown by detailed investigations that it can never be possible to obtain satisfactory agreement with empirical values under the limitation of one meson emission* (*or first order perturbation calculations*) because of too large values of anomalous magnetic moments of nucleons and very large mass value of π-meson. This is the conclusion (i).

§ 3. Two mesons emission

In this case, there are three possible virtual states :

$$\begin{aligned} &\text{for Proton ; } \quad P(+1/2);\ N(-1/2)+\pi^+(+1);\ P(+1/2)+\pi^+(+1)+\pi^-(-1), \\ &\text{for Neutron ; } N(+1/2);\ P(-1/2)+\pi^-(+1);\ N(+1/2)+\pi^-(+1)+\pi^+(-1). \end{aligned} \tag{5}$$

Let a and β be the fraction of time in which one meson and two mesons are emitted. The magnetic moments are given by the following formulae :

$$\begin{aligned} \mu_P &= 1-a-\beta+a(M/m^*)+\beta+2\beta(M/m^*), \\ \mu_N &= -a-a(M/m^*)-2\beta(M/m^*), \end{aligned} \tag{6}$$

where the effective mass of π-meson is assumed to be the same for all virtual states. Here it is to be remarked that the meson current contributions (i.e., the terms containing

m^*) are of the same of magnitude and of opposite sign for a proton and a neutron, which is the case in exact fourth order calculations[2]. Further this situation is the same in previous case (2) (i.e., second order calculations) and in all the following cases including cases of excited states. Thus the value of $\mu_P+\mu_N$ determines a relation between α and β (and γ (see in the following)) irrespective of the values of m^*. In this case one obtains

$$\mu_P+\mu_N=1-2\alpha=0.8793, \tag{7}$$

from which one obtains quite the same value as in § 2:

$$\alpha=0.0604. \tag{8}$$

From the value of $\mu_P-\mu_N$, we obtain, if $m^*\geq 276m_e$,

$$\beta\geq 0.1086. \tag{9}$$

Thus we can say that the inclusion of virtual states of two mesons present improves the situation very much and it is possible to adjust the parameters α, β and m^* to fit μ_P and μ_N. However the choice of parameter $\beta(\fallingdotseq 2\alpha)$ is not quite reasonable from physical considerations: the neglect of higher order corrections becomes very doubtful. *Therefore it seems to the author that the quite satisfactory agreement cannot be attained by the fourth order perturbation calculations.* These are the conclusion (ii).

§ 8. Three or more mesons emission

If we include virtual states of three mesons present in addition to those in (5), namely

$$\begin{aligned} &\text{for Proton;} \quad N(-1/2)+\pi^+(+1)+\pi^-(-1)+\pi^+(+1),\\ &\text{for Neutron;} \quad P(-1/2)+\pi^-(+1)+\pi^+(-1)+\pi^-(+1), \end{aligned} \tag{10}$$

we obtain, γ being the fraction of time in which three mesons are emitted,

$$\begin{aligned} \mu_P&=1-\alpha-\beta-\gamma+\alpha(M/m^*)+\beta+2\beta(M/m^*)+3\gamma(M/m^*),\\ \mu_N&=-\alpha-\alpha(M/m^*)-2\beta(M/m^*)-\gamma-3\gamma(M/m^*), \end{aligned}$$

from which one readily obtains

$$\begin{aligned} &\alpha+\gamma=0.0604,\\ &2\alpha+4\beta+6\gamma\geq 0.5550, \quad \text{if } m^*\geq 276\mathrm{m}_e. \end{aligned} \tag{11}$$

From above equations, it follows

$$\alpha+\gamma=0.0604 \quad \text{and} \quad \beta+\gamma\geq 0.1086, \tag{12}$$

which means that the inclusion of a term proportional to γ makes the ratio β/α larger than in the case $\gamma=0$; this seems to the author to be undesirable and it is concluded that it seems hopeless to get better agreement with empirical values by simply carrying out further perturbation calculations, which is the conclusion (iii).

§ 5. Neglect of decrease of normal magnetic moment

If we do not take into account the decrease of the normal part of magnetic moment of proton caused by the meson clouds around it, we obtain in the case of two π-mesons emission

$$\begin{aligned} \mu_P &= 1+\alpha(M/m^*)+\beta+2\beta(M/m^*), \\ \mu_N &= -\alpha-\alpha(M/m^*)-2\beta(M/m^*), \end{aligned} \tag{13}$$

from which one obtains, $m^* \geq 276 m_e$,

$$\alpha \geq 0.167\,; \quad \beta \geq 0.047. \tag{14}$$

Above values are quite different from those in (8) and (9), indicating that neglect of these modifications has very large effect on the values of magnetic moments and the completely satisfactory adjustment of parameters is possible simply by adding the virtual states of two mesons present in this case, which is the conclusion (iv).

§ 6. Inclusion of excited state of $\sigma=3/2$ and $\tau=3/2$

If in the state of two mesons present, for example $P(1/2)+\pi^+(+1)+\pi^-(-1)$, π^+ meson may interact strongly with $P(1/2)$ and they may form an excited state $P^+(3/2)$, whose charge is $+2e$ and whose angular momentun is $+3/2$, we then obtain a virtual state in which $P(1/2)$ is excited to $P^+(3/2)$ accompanied by $\pi^-(-1)$ emission. Likewise for neutron $N(1/2)$, we obtain a virtual state in which $N(1/2)$ is excited to $N^-(3/2)$, which is not an anti-proton but a negatively charged nucleon, accompanied by $\pi^+(-1)$ emission. Let δ be the fraction of time of above transition. If we consider α, β and δ, we obtain

$$\begin{aligned} \mu_P &= 1-\alpha-\beta-\delta+\alpha(M/m^*)+\beta+2\beta(M/m^*)+6\delta+\delta(M/m^*), \\ \mu_N &= -\alpha-\alpha(M/m^*)-2\beta(M/m^*)-3\delta-\delta(M/m^*), \end{aligned} \tag{15}$$

from which we obtain following sets of values, for example, for $m^* \geq 276 m_e$;

$$\begin{aligned} &\text{(i)} \quad \alpha \geq 0.08, \quad \beta \geq 0.08, \quad \delta \geq 0.02, \\ &\text{(ii)} \quad \alpha \geq 0.10, \quad \beta \geq 0.06, \quad \delta \geq 0.04, \\ &\text{(iii)} \quad \alpha \geq 0.14, \quad \beta \geq 0.00, \quad \delta \geq 0.08. \end{aligned} \tag{16}$$

From these figures one can conclude that by including above excited state the ratio β/α can be reduced as much as we want, thus the completely satisfactory adjustment of parameters is possible only if we permit small value for δ. Further it is to be remarked that it is also possible to make β vanish completely (see above assignment (iii)) and also to eliminate α (the conventional virtual π-meson emission) entirely because we may as well consider the nucleon $N(-1/2)$ (or $P(-1/2)$) in the virtual state as nothing but the nucleon whose spin and τ-spin are both $3/2$ but are inclined in their directions with respect to the directions of spin and τ-spin of original nucleon. Thus we can explain the

magnetic moments phenomenologically at least in terms of virtual transition of an original nucleon to its excited state of spin 3/2 and τ-spin 3/2. Now it is clear that the inclusion of above mentioned excited state is essential and the usual transition accompanied by one or two mesons emission may be modified quite arbitrarily and can be made vanished without affecting the situations at all. These are the conclusion (v) and the most important one in this paper. It must be added that the great success in this case results entirely from the large nucleon magnetic moments of doubly charged nucleon $P^+(3/2)$ and negatively charged nucleon $N^-(3/2)$.

§ 6. Inclusion of excited state of $\sigma=3/2$, $\tau=1/2$, or $\sigma=1/2$, $\tau=3/2$

In order to show the importance of the excited state of $\sigma=3/2$ and $\tau=3/2$, we shall investigate other excited states of $\sigma=3/2$, $\tau=1/2$ and $\sigma=1/2$, $\tau=3/2$. In both cases it is readily seen that the inclusion of possible virtual states under the restrictions imposed in the first section makes worse the situation on the contrary, because such states are for the two cases respectively

$$\begin{aligned} &N(3/2)+\pi^+(-1), \quad N(-1/2)+\pi^+(+1), \\ \text{and}\quad &P^+(-1/2)+\pi^-(+1), \quad N(-1/2)+\pi^+(+1). \end{aligned} \tag{17}$$

Then we remove the above restrictions temporarily and pick up the most favorable virtual states to the magnetic moments of nucleons, which are for a proton $P(+1/2)$

$$\begin{aligned} &\text{in case of } \sigma=3/2,\ \tau=1/2\,;\ P(3/2)+\pi^\circ(-1) \text{ and } N(-3/2)+\pi^+(+2), \\ &\text{in case of } \sigma=1/2,\ \tau=3/2\,;\ P^+(1/2)+\pi^-(\mathrm{o}). \end{aligned} \tag{18}$$

In the former case, we get quite in the same way as before the following relations between α, β, δ and m^*;

$$\begin{aligned} &\alpha+\delta=0.0604, \\ &4\delta+(2\alpha+4\beta+4\delta)M/m^*=3.6999, \end{aligned} \tag{19}$$

from which for $m^*\geq 276\ m_e$

$$\begin{aligned} &\text{(i)} \quad \alpha=\delta=0.0302, \quad \beta\geq 0.0889, \\ &\text{(ii)} \quad \alpha=0,\ \delta=0.0604,\ \beta\geq 0.0743. \end{aligned} \tag{20}$$

Thus it is impossible to diminish β and there is no reasonable adjustment of parameters in this case. In the latter case we get

$$\begin{aligned} &\alpha=0.0604, \\ &2\delta+(2\alpha+4\beta)M/m^*=3.6999, \end{aligned} \tag{21}$$

which gives $\beta\geq 0.1040$ if $m^*\geq 276m_e$ for $\delta=\alpha=0.0604$, which is almost the same value as (9). Thus it is again impossible to diminish β. It is here to be remarked that the assumed virtual states (18) are even unreasonable from theoretical considerations. Now

it is concluded that the inclusion of other excited state, namely, of $\sigma=3/2$ and $\tau=1/2$ or of $\sigma=1/2$ and $\tau=3/2$, does not improve the situation at all. Therefore the inclusion of an excited state of $\sigma=3/2$ and $\tau=3/2$ is definitely required. These are the final conclusion (vi).

§ 8. Discussions about the excited state of $\sigma=3/2$, $\tau=3/2$

By the preceding investigations was made clear the inevitability of assuming the nucleon excited state of $\sigma=3/2$ and $\tau=3/2$ in order to fit the magnetic moments of nucleons. Now we shall discuss about the nature of this excited state.

As was mentioned in the introduction, it may either be considered as the all-inclusive estimation of higher order corrections, or imply a modification of the present theory which is equivalent to give a nucleon another new freedom which prescribes whether the nucleon is in its ground state or in its excited state. In order to decide these we must rely upon the exact theoretical investigations, which are now in preparation. However it seems to the author that the latter standpoint turns out to be the case because, as is discussed in § 4, it seems hopeless to get better agreement with empirical values by simply carrying out successive perturbation calculations and therefore even the summary estimation of all higher order corrections may not suffice to get the satisfactory agreement with empirical values. The next work is therefore to carry out exact calculations in which the present theory is modified to include the above mentioned new freedom. Also it is interesting to see whether the anomalies observed in proton-proton scattering can be explained along these lines or not.

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References

1) J. M. Luttinger, Phys. Rev. **75** (1949), 309.
M. Slotnick and W. Heitler, Phys. Rev. **75** (1949), 1645.
K. M. Case, Phys. Rev. **76** (1949), 1.
2) K. Nakabayasi and I. Sato, Prog. Theor. Phys. **6** (1951), 252.
3) K. A. Brueckner, Phys. Rev. **86** (1952), 106.

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Photodisintegration of the Deuterons at High Energies

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The effect of tensor forces in the photodisintegration of deuterons are investigated. The calculation shows that the angular distribution can be given in the form $\{a+(b+c\cos\theta)\sin^2\theta+d\cos\theta\}$ and no other additional terms appear.

§ 1. Introduction

Our knowledge on the nuclear forces has been supplied mainly from neutron-proton and proton-proton scattering experiments. As the conclusion thereof, two different views have been proposed. One of which, introduced by Serber, assumes no forces between nucleons if they are in P-states or odd states each other. This type of potential is first proposed to explain the angular distribution in neutron-proton scatterings. However, it fails to give the large scattering probabilities and the angular distribution of proton-proton scattering at high energies. On the last point, Jastrow[1] has removed the difficulties by introducing hard core in the singlet states. But the existence of hard core makes the effective range somewhat longer and thus one must take shorter intrinsic range than that inferred from the current meson theories.

The second view, proposed by Christian and Noyes[2], assumes, on the contrary, strong tensor forces between nucleons in P-states. This potential has first been introduced to give the flat angular distribution of high energy proton-proton scattering. Recently Matuzaki and the author[3] have applied this potential to calculate the π^+-meson capture process by deuterons and obtained better results as well in the energy dependence of the probabilities as in the angular distribution of the emitted protons. Although this type of potential is originally limited to the forces between neutron and proton, it will be interesting to extend it to the case of neutron-proton forces, following the concept of charge independence of nuclear forces. For that purpose a little modification will be needed. As is well known, the force in P-state causes generally asymmetric scattering around 90°, i.e., when the force is repulsive, backward and when it is attractive, forward scattering. Thus, according to Taketani's suggestion,[4] we assume hard core with singular tensor force, which then will reduce the phase shifts in S-state and cause the scattering to become forward even for exchange forces. The situation is the same as in the case of Jastrow's potential. The sum of scattering due to triplet and singlet states will therefore almost symmetric around 90°. This balancing seems to prevail in the wide range of energies[5].

The assumption of strong forces in P-states will also results in the change of transition probabilities in the other various processes. We shall here investigate the photodisintegration of deuterons.

The experiments on the photo-process of deuterons have recently been made in the various ranges of energies. In the lower energy region, Krohn and Schrader[6] and others have performed the experiments using 5～17 MeV gamma rays. Their results can be written in the form:

$$d\sigma \sim \{a+(b+c\cos\theta)\sin^2\theta\}. \tag{1}$$

Here a represents the spherically symmetric part. The values of a are at variance according to the authors and vary from 0.07 to $0.2b$. This part of distribution comes from magnetic dipole transition, when gamma ray energies are sufficiently low. The probabilities of this transition, however, decrease rapidly with increasing gamma ray energies and become negligibly small, while the experimental results do not indicate remarkable decrease, or rather show small increase.

In the high energy range, Benedict and Woodward, Littauer and Keck and others[7] have investigated the angular distribution of the process. Their results can also be written as (1) and according to Benedict and Woodward, $a \sim c \sim 0.4b$ for gamma ray energy of 165 MeV.

These results show that the spherical part a is not due to magnetic transitions. In the electric dipole transitions the angular distribution is proportional to $\sin^2\theta$, when only central forces are present in the ^1P-state. However, if non-central forces are exerted, the spherical symmetric part will step in besides. This is because the phases as well as the magnitudes of transition matrix elements become different and the interferences between them are changed.

Although the experiments in the energy range of 20～100 MeV have not yet been made and thus no definite conclusions may be deduced from this process, we are giving here the general formula to determine the angular distribution of the photodisintegration process for the future purpose.

§ 2. Differential cross sections

According to Schwinger[8] the differential cross section of the photodisintegration due to electric dipole and quadrupole transitions is given by

$$d\sigma(\theta) \sim \frac{e^2}{\hbar c}\frac{\hbar\omega}{Mc^2}\left(\frac{Mc}{\hbar}\right)^2 k \frac{1}{3}\sum_{m,m'}\left|\bar{\Psi}_f\left(\frac{r}{2}(\boldsymbol{e}\boldsymbol{r})+i\frac{\omega r^2}{8c}(\boldsymbol{e}\boldsymbol{r})(\boldsymbol{\varkappa}\boldsymbol{r})\right)\Psi_i\right|^2 \frac{d\Omega}{4\pi}\ ^{*)}. \tag{2}$$

Here $\hbar\omega$ is the energy of the incident photons which come in the direction of $\boldsymbol{\varkappa}$ with the polarization direction $\boldsymbol{e}$, and Ψ_i, Ψ_f are the wave functions of initial and final states of neutron-proton system. When tensor forces exist, the initial wave function Ψ_i is the mixture of S and D states and is given symbolically as:

$$\bar{\Psi}_i = (4\pi)^{-\frac{1}{2}}\left\{\frac{u(r)}{r}+2^{-\frac{3}{2}}S_{12}\frac{w(r)}{r}\right\}\chi_1^m \tag{3}$$

*) Gothics always represent unit vectors.

where $u(r)$ and $w(r)$ are radial function of S and D states, χ_1^m is the triplet spin function whose z-component is m and S_{12} is tensor operator,

$$S_{12}=3(\sigma_1 r)(\sigma_2 r)-(\sigma_1\sigma_2). \tag{4}$$

The final wave function Ψ_f is expanded into series of spherical harmonics,

$$\Psi_f=\sum_{J,l}(2l+1)i^l\cdot\exp[-i\delta_l^J]\frac{u_l^J(r)}{kr}O_l^J P_l(\cos\theta)\,\chi_1^m \tag{5}$$

where O_l^J is the projection operators which separate the states with different total angular momentum J in l-states.

As the ground state of deuteron consists of the mixture of S and D states, the transitions take place to the states :

electric dipole : $\quad {}^3P_0, \quad {}^3P_1, \quad {}^3P_2,$

electric quadrupole : $\quad {}^3S_1+{}^3D_1, \quad {}^3D_2, \quad {}^3D_3.$

Therefore it will be sufficient to consider only S, P and D-waves in the final states. The mixed waves ${}^3S+{}^3D$ in the final states are complex, i.e., the one in which S wave is dominant and that, where D wave is dominant. However, we need not distinguish between them in the general formulation.

First the projection operator O_l^J must be constructed. As the problem is restricted to the triplet states, only such parts of spin matrices,

$$\boldsymbol{S}=\frac{1}{2}(\sigma_1+\sigma_1) \tag{6}$$

that have eigenvalue unity, are needed. It can easily be shown that such reduced matrices are represented by the well-known rotation matrices :

$$S_x=\begin{pmatrix}0&0&0\\0&0&-i\\0&i&0\end{pmatrix},\quad S_y=\begin{pmatrix}0&0&i\\0&0&0\\-i&0&0\end{pmatrix},\quad S_z=\begin{pmatrix}0&-i&0\\i&0&0\\0&0&0\end{pmatrix}. \tag{7}$$

These matrices satisfy the following relations :

$$\begin{aligned}&\boldsymbol{S}\times\boldsymbol{S}=i\boldsymbol{S},\\&S_iS_jS_k+S_kS_jS_i=\delta_{ij}S_k+\delta_{kj}S_i,\\&S_iS_j(S^2_k-1)=0\end{aligned} \tag{8}$$

which will be conveniently employed in the calculation.

For the states with angular momentum $\boldsymbol{l}=\frac{1}{i}(\boldsymbol{r}\times\boldsymbol{\nabla})$, total spin $\boldsymbol{S}$ and total angular momentum $\boldsymbol{J}=\boldsymbol{l}+\boldsymbol{S}$, the eigenvalues of $(\boldsymbol{lS})$ are well defined and are given by

$$(\boldsymbol{lS})=\frac{1}{2}\{J(J+1)-l(l+1)-S(S+1)\}. \tag{9}$$

In our system the states are divided into three, $J=l\pm1$ and $J=l$, as $S=1$. Because $(\boldsymbol{lS})$ has different eigenvalues for the states with different J(and equal l), we can employ this

operator to construct the projection operators O_l^J; they are

$$\begin{aligned}
&\text{for } P\text{-state} \quad J=0 \quad \frac{1}{3}\{(\boldsymbol{lS})^2-1\},\\
&\qquad\qquad J=1 \quad -\frac{1}{2}\{(\boldsymbol{lS})-1\}\{(\boldsymbol{lS})+2\},\\
&\qquad\qquad J=2 \quad \frac{1}{6}\{(\boldsymbol{lS})+1\}\{(\boldsymbol{lS})+2\},\\
&\text{for } D\text{-state} \quad J=1 \quad \frac{1}{10}\{(\boldsymbol{lS})-2\}\{(\boldsymbol{lS})+1\},\\
&\qquad\qquad J=2 \quad -\frac{1}{6}\{(\boldsymbol{lS})-2\}\{(\boldsymbol{lS})+3\},\\
&\qquad\qquad J=2 \quad -\frac{1}{15}\{(\boldsymbol{lS})+1\}\cdot\{(\boldsymbol{lS})+3\}.
\end{aligned} \tag{10}$$

Now we operate O_l^J on $P_1(\cos\theta)$ and $P_2(\cos\theta)$, then the separated parts of the partial waves are obtained:

$$\begin{aligned}
&\text{for } P\text{-state} \quad J=0 \quad \frac{1}{3}\{(\boldsymbol{kr})-(\boldsymbol{Sk})(\boldsymbol{Sr})\},\\
&\qquad\qquad J=1 \quad \frac{1}{2}(\boldsymbol{Sr})(\boldsymbol{Sk}),\\
&\qquad\qquad J=2 \quad \frac{1}{6}\{2(\boldsymbol{Sk})(\boldsymbol{Sr})-3(\boldsymbol{Sr})(\boldsymbol{Sk})+4(\boldsymbol{kr})\},\\
&\text{for } D\text{-state} \quad J=1 \quad \frac{1}{12}S_{12}\{(\boldsymbol{Sk})^2-\frac{2}{3}\},\\
&\qquad\qquad J=2 \quad -\frac{1}{6}[S_{12}\{(\boldsymbol{Sk})^2-\frac{2}{3}\}+4(\boldsymbol{kr})[(\boldsymbol{Sk})(\boldsymbol{Sr})]\\
&\qquad\qquad\qquad\qquad -4\{(\boldsymbol{kr})^2-\frac{1}{3}\}],\\
&\qquad\qquad J=3 \quad \frac{1}{15}[S_{12}\{(\boldsymbol{Sk})^2-\frac{2}{3}\}+10(\boldsymbol{kr})[(\boldsymbol{Sk}),(\boldsymbol{Sr})]\\
&\qquad\qquad\qquad\qquad +5\{(\boldsymbol{kr})^2-\frac{1}{3}\}].
\end{aligned} \tag{11}$$

As the waves are separated, the matrix elements for the photo-process can be obtained straightforward. The matrix element for the electric dipole transition is, after the integration with respect to the radial part $\boldsymbol{r}$,

$$-i(4\pi)^{-\frac{1}{2}}\cdot\frac{3}{2}\chi_1^m(\boldsymbol{er})[\frac{1}{3}\exp(-i\delta_1^0)\{(\boldsymbol{kr})-(\boldsymbol{Sr})(\boldsymbol{Sk})\}I_0$$

$$+\frac{1}{2}\exp(-i\delta_1^1)2(\boldsymbol{Sk})(\boldsymbol{Sr})I_1+\frac{1}{6}\exp(-i\delta_1^2)\{2(\boldsymbol{Sr})(\boldsymbol{Sk})$$

$$-3(\boldsymbol{Sk})(\boldsymbol{Sr})+4(\boldsymbol{kr})]I_2]\chi_1^{m'}\,d\Omega_r\,, \tag{12}$$

$$I_0=\frac{1}{k}\int rv_0(u-2^{\frac{1}{2}}w)\,dr,\quad I_1=\frac{1}{k}\int rv_1(u+2^{\frac{1}{2}}w)\,dr, \tag{13}$$

$$I_2=\frac{1}{k}\int rv_2(u-\frac{1}{5}2^{-\frac{1}{2}}w)\,dr$$

where v_0, v_1 v_2, are the radial functions for $J=0$, 1 and 2 states, respectively. For the transition from D ground state to P, the tensor operator S_{12}, operated on the states of $J=0$, 1, 2, gives the factors 4, 2, 2/5 and thus the integrals are only multiplied by these factors. The operator S_{12} has non-diagonal element besides and gives rise to the transition to ${}^3F_2$ state when operated on ${}^3P_2$ state. However, its transition matrix element vanishes, after the integration over the solid angle of space coordinates, thus that part of the matrix element is omitted here.

The integration over the solid angle of space gives

$$\begin{aligned}-i(4\pi)^{\frac{1}{2}}\cdot\frac{1}{2}\cdot\chi_1^m[&\frac{1}{3}\exp(-i\delta_1^0)\{(\boldsymbol{ke})-(\boldsymbol{Se})(\boldsymbol{Sk})\}I_0\\&+\frac{1}{2}\exp(-i\delta_1^4)\cdot(\boldsymbol{Sk})(\boldsymbol{Se})I_1+\frac{1}{2}\exp(-i\delta_1^2)\{\frac{2}{3}(\boldsymbol{Se})(\boldsymbol{Sk})\\&-(\boldsymbol{Sk})(\boldsymbol{Se})+\frac{4}{3}(\boldsymbol{ke})\}I_2]\chi_1^m.\end{aligned} \tag{14}$$

Analogously, the expression for the electric quadrupole transition can be obtained. Here we treat the transitions to ${}^3D$ and ${}^3S$ separately. For the transition to ${}^3S$,

$$i(4\pi)^{\frac{1}{2}}\frac{\omega}{8c}\cdot 2^{-\frac{3}{2}}\cdot\frac{1}{5}\chi_1^m\{(\boldsymbol{eS})(\boldsymbol{kS})+(\boldsymbol{kS})(\boldsymbol{eS})\}L\chi_1^{m'} \tag{15}$$

with

$$L=\frac{1}{k}\int u_1 w\,dr \tag{16}$$

where u_1 is the radial function for the final S-state. And for the transition to D:

$$\begin{aligned}-i(4\pi)^{\frac{1}{2}}\frac{5\omega}{8c}\chi_1^{m'}[&\frac{1}{50}\exp(-i\delta^1{}_2)AJ_1-\frac{1}{30}\exp(-i\delta_2^2)\{A+\frac{2}{3}B-\frac{4}{3}(\boldsymbol{ek})(\boldsymbol{\varkappa k})\}J_2\\&+\frac{1}{15}\exp(i\delta_2^3)\{\frac{1}{5}A+\frac{1}{3}B+\frac{1}{3}(\boldsymbol{ek})(\boldsymbol{\varkappa k})\}J_3]\chi_1^{m'}\end{aligned} \tag{17}$$

with

$$A=\{(\boldsymbol{Sk})^2-\frac{2}{3}\}\cdot\{(\boldsymbol{Se})(\boldsymbol{Sk})+(\boldsymbol{Sk})(\boldsymbol{Se})\},\quad B=[\{(\boldsymbol{Se})(\boldsymbol{k\varkappa})+(\boldsymbol{S\varkappa})(\boldsymbol{ke})\},(\boldsymbol{Sk})] \tag{18}$$

and

$$J_1=\frac{1}{k}\int u^2 w_1\cdot(u-2^{-\frac{1}{2}}w)dr,\ J_2=\frac{1}{k}\int r^2 w_3(u+2^{-\frac{1}{2}}w)dr,$$

$$J_3=\frac{1}{k}\int r^2 w_3(u-\frac{1}{7}2^{\frac{1}{2}}w)dr \tag{19}$$

where w_1, w_2, w_3 are the radial function for $J=1,2$, and 3. For the transitions from D ground state we have only to multiply the expression for those from S ground state by the factor -2, 2 and $-4/7$. As the operator S_{12} has non-diagonal elements, ${}^3S_1$ and ${}^3G_3$ terms also appear when operated on ${}^3D_1$ and ${}^3D_3$, respectively. However, these nondiagonal transitions vanish again, if integrated over the solid angle.

To obtain the transition probabilities, we have to take the absolute squares of the matrix elements and sum up with respect to the spin directions of the initial and final states. In this procedure the calculations can be simplified as follows. Let A and B be arbitrary functions of spin matrices $\boldsymbol{S}$, then the orthogonality of spin functions gives the relation :

$$\sum_{m,m'}\chi_1^m A\chi_1^{m'}\cdot\chi_1^{m'} B\chi_1^m=\sum_m\chi_1^m A\cdot B\,\chi_1^m=Sp\ AB. \tag{20}$$

With this relation we have for the electric dipole transition probability,

$$\frac{\pi}{3}\frac{e^2}{\hbar c}\cdot\frac{M\omega}{\hbar k}\Big[\frac{1}{9}I_0^2+\frac{3}{9}I_1^2+\frac{5}{9}I_2^2$$

$$-\frac{1}{72}(3\cos^2\theta-1)\{3I_1^2+7I_2^2+8I_0I_2\cos(\delta_1^0-\delta_1^2)+18I_1I_2\cos(\delta_1^1-\delta_1^2)\}\Big]. \tag{21}$$

This expression is the same with those obtained by Schwinger. For the interference between dipole and quadrupole transitions, we have two separated parts ; one of which is the interference of electric dipole with the transition to ${}^3S$ final state and the other is that with the transition to D final state. They are :

$$\frac{\pi}{60\sqrt{2}}\cdot\frac{e^2}{\hbar c}\cdot\frac{M\omega^2}{k\hbar c}\Big[\frac{1}{3}I_0\cos(\delta_0^1-\delta_1^0)-\frac{1}{2}I_1\cos(\delta_0^1-\delta_1^1)+\frac{1}{6}I_2\cos(\delta_0^1-\delta_1^2)\Big]L\cos\theta, \tag{22}$$

and

$$\frac{\pi}{54}\cdot\frac{e^2}{\hbar c}\cdot\frac{M\omega^2}{k\hbar c}\Big[\frac{1}{5}I_0J_1\cos(\delta_1^0-\delta_2^1)+\frac{3}{20}I_1J_1\cos(\delta_1^1-\delta_2^1)+\frac{1}{4}I_2J_1\cos(\delta_1^2-\delta_2^1)$$

$$+\frac{7}{12}I_1J_2\cos(\delta_1^1-\delta_2^2)+\frac{5}{12}I_2J_2\cos(\delta_1^2-\delta_2^2)+\frac{2}{15}I_0J_3\cos(\delta_1^0-\delta_2^3)$$

$$+\frac{4}{15}I_1J_3\cos(\delta_1^1-\delta_2^3)+I_2J_3\cos(\delta_1^2-\delta_2^3)$$

$$-(3\cos^2\theta-1)\{\frac{3}{10}I_0J_1\cos(\delta_1^2-\delta_2^1)+\frac{1}{6}I_1J_2\cos(\delta_1^1-\delta_2^2)+\frac{1}{3}I_2J_3\cos(\delta_1^2-\delta_2^2)$$

$$+\frac{1}{6}I_0J_3\cos(\delta_1^0-\delta_2^3)+\frac{1}{3}I_1J_3\cos(\delta_1^1-\delta_2^3)+\frac{1}{5}I_2J_3(\delta_1^2-\delta_2^3)\}\Big]\cos\theta. \tag{23}$$

The electric quadrupole transitions are separated into three, the square of the transition to

S final state, the cross term of the transitions to S and D finals, and the square of the transition to D state. They are,

$$\frac{\pi}{4800}\frac{e^2}{\hbar c}\frac{M\omega^3}{k\hbar c^2}L^2, \tag{24}$$

$$\frac{\pi}{1440\sqrt{2}}\frac{e^2}{\hbar c}\frac{M\omega^3}{k\hbar c^2}\left[\frac{1}{10}J_1\cos(\delta_2^1-\delta_0^1)-\frac{1}{6}J_2\cos(S_2^2-\delta_0^1)\right.$$
$$\left.+\frac{1}{15}J_3\cos(\delta_2^3-\delta_0^1)\right](3\cos^2\theta-1)L, \tag{25}$$

and

$$\frac{\pi}{64800}\cdot\frac{e^2}{\hbar c}\cdot\frac{N\omega^3}{k\hbar c^2}\left[\frac{3}{4}(3\cos^2\theta+7)J_1^2+\frac{5}{12}(-16\cos^4\theta+15\cos^2\theta+3)J_2^2\right.$$
$$+\frac{1}{3}(-55\cos^4\theta+78\cos^2\theta+27)J_3^2+\frac{5}{2}(3\cos^2\theta+1)J_1J_2\cos(\delta_2^1-\delta_2^2)$$
$$+\frac{2}{3}(-25\cos^4\theta+24\cos^2\theta-3)J_2J_3\cos(\delta_2^2-\delta_2^3)$$
$$\left.+2(-45\cos^4\theta+39\cos^2\theta-2)J_3J_1\cos(\delta_2^3-\delta_2^1)\right] \tag{26}$$

respectively. Here the last expression is the largest, while the other two give only negligibly small contributions.

§ 3. Application to the pseudoscalar meson potential

The final results are considerably complicated and one could not deduce general feature of the effects due to tensor forces. Thus we shall here see the tendency by applying the formulae to the pseudoscalar meson potential, which has strong tensor forces. As the potential has $1/r^3$ singularity, the cutoff procedure must be used to avoid the divergence difficulties. In our case, according to Taketani, the hard core cutoff has been employed. Then the potential is

$$V(x)\sim\varkappa g^2\cdot\frac{1}{3}(\tau_1\cdot\tau_2)\left\{\frac{1}{3}+\left(\frac{1}{x^2}+\frac{1}{x}+\frac{1}{3}\right)S_{12}\right\}\frac{e^{-x}}{x},\quad\text{for } x\geq x_0,\ (x=\varkappa r).$$

The constants for this potential have been calculated by Onuma[9] and they are $1/\varkappa=1.406\times10^{-13}cm$, $\varkappa g^2=35.5MV$ and the cutoff radius x_0 is 0.458. With these values the potential gives the cosistent results for the ground state of deuterons and low energy state of neutron-proton system. As we are interested in the case where the forces exist even in P state, the symmetrical theory is considered. Then the forces are strongly attractive in $^3P_2$, strongly repulsive in $^3P_1$, and weakly attractive in $^3P_2$, while in D-state the forces are strong repulsion in $^3D_1$, comparatively attraction in $^3D_2$, and weak repulsion in $^3D_3$. There are general tendencies that the transition matrix elements have large values when in the final states the forces are repulsive and smaller values for an attractive forces in the final states. In our case the transition to $^3P_1$ state has large value and thus as the tensor force increases, the spherical part in the angular distributions increases. The interference

between electric dipole and quadrupole transitions gives generally $\cos\theta\cdot\sin^2\theta$ distribution and thus somewhat forward emission. With increase of tensor force the repulsion in ${}^3P_1$ and ${}^3D_1$ become dominant and the distribution proportional to $\cos\theta$ appears besides. This terms gives considerably different distribution from that expected from usual photo-process, but in general has small values, unless unusually singular potential is used. Therefore, this term will remain always as small correction.

The calculation have been made for $\hbar\omega=150$ MeV. The phase shifts are estimated by Born approximation and for the radial function of ground state, only S wave is considered, which form is taken from that of Hulthén. This simplification corresponds to the neglect of hard core. The angular distribution can then be written as:

$$d\sigma\sim\{a+(b+c\cos\theta)\ \sin^2\theta+d\cos\theta\} \tag{27}$$

with $a\sim c\sim 0.3b$. The ratio seems to remain unchanged in the wide range of energies. The term proportional to $\cos\theta$ is small by the factor more than 10, and gives no remarkable contribution to the distribution. This result can be compared with the experimental values obtained by Benedict and Woodward. However, the almost flat distribution obtained by Littauer and Keck would not be attained, whatever potential one may choose.

§ 4. Conclusion

We have calculated the formula to give the angular distribution of photo-process of deuterons, when non-central forces are present. The spherical part of the distribution comes from electric dipole transitions, while the interference between electric dipole and quadrupole transitions gives no modification anew. Therefore, the general form of the distribution will be given by (27).

The total cross section of the photo-process behaves as that calculated by usual theory so long as the gamma ray energies are less than 100 MeV. The experimental results show, however, strong increase for the energies higher than that. In our case the agreement is elongated up to 150 MeV because of the forces in P-states, and after that the cross section becomes almost flat. Therefore some modification will be needed for the higher energy regions, to explain the increase, and the validity of our form (27) must be limited to the energy range below 100 or 150 MeV.

References

1) R. Jastrow, Phys. Rev. **81** (1951), 165.
2) R. S. Christian and H. P. Noyes, Phys. Rev. **79** (1950), 95.
3) Y. Matuzaki and M. Sasaki, Prog. Theor. Theor. Phys. **7** (1952), 573.
4) M. Taketani, S. Nakamura and M. Sasaki, Prog. Phys. **6** (1951), 581.
5) Y. Matuzaki and M. Sasaki (to be published in this issue).
6) V. F. Krohn, Jr. and E. F. Schrader, Phys. Rev. **86** (1951), 391.
7) T. S. Benedict and W. M. Woodward, Phys. Rev. **85** (1952), 924: W. S. Gilbert and J. W. Rose, Phys Rev. **85** (1952), 766: S. Kikuchi, Phys. Rev. **85** (1952), 1062: R. Littauer and J. Keck, Phys. Rev. **86** (1952), 1051.
8) W. Rarita and J. Schwinger, Phys. Rev. **59** (1941), 556: N. Austern, Phys. Rev. **85** (1952), 283.
9) M. Taketani, S. Machida and S. Onuma, Prog. Theor. Phys. **7** (1952), 45.

Letters to the Editor

Principle of Detailed Balance in Quantum Field Theory

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1. Principle of detailed balance

Recently an interesting discussion has been given by F. Coester about Heitler's conjecture, that the principle of detailed balance holds generally if averages over the spin variables are taken, even if it may not be expected to hold in quantum theory in general. The above circumstances were proved for the first time by Hamilton and Peng in a concrete example and recently by F. Coester in a more general form using Wigner's operator of time reversal. The purpose of this note is to show that the principle of detailed balance holds rigorously in the present relativistic quantum field theory.

The inverse process of a given process may be interpreted as that whose events occur in the order of increasing t' in the coordinate system $x'=-x$, $t'=-t$ with reversed space and time directions, the corresponding momenta and spins being effectively invariant (see the figure and the paragraph 2). By this inversion procedure, not only classical collision diagrams but also quantum field theoretical Feynman-Dyson's diagrams become those which have the same configuration and the inversed order of events.

Hamiltonians in the interaction representation take relativistic invariant or pseudoscalar forms, so they remain invariant also under space-time inversion for spinors and tensors build up representations of the whole Lorentz group. For example, in the case of electron-photon system Hamiltonian is

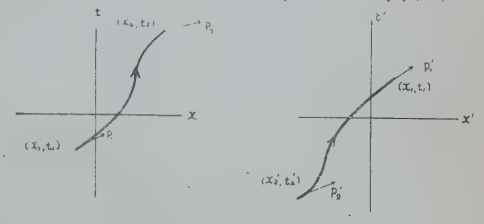
$$H_{ep}=-ie\bar{\psi}\gamma_\mu\psi A_\mu-\delta_m c^2\bar{\psi}\psi,$$

and in the case of nucleon- meson-photon system

$$H_{nmp}\frac{ie}{\hbar c}\left(\bar{\varphi}\frac{\partial\varphi}{\partial\chi^\mu}-\frac{\partial\bar{\varphi}}{\partial\chi^\mu}\varphi\right)A_\mu$$

$$-\left(\frac{ie}{\hbar c}\right)^2\bar{\varphi}\varphi A_\mu A_\mu+ic(\bar{\Psi}\gamma_\mu\tau_p\Psi)A_\mu$$

$$+if\bar{\Psi}\gamma_5(\tau_-\bar{\varphi}+\tau_+\varphi)\Psi+\delta_\lambda(\bar{\varphi}\varphi)^2,$$



where A_μ is the photon field (vector), ψ the electron field (spinor), Ψ the nucleon field (spinor), φ the meson field (scalar or pseudo scalar). Under the coordinate transformation

$$x'=-x,\quad t'=-t, \tag{1}$$

these fields transform as follows

$$A_\mu'=-A_\mu,\ \varphi'=\varphi,\ \psi'=T\psi,\ \Psi'=T\Psi$$

where

$$T=\begin{pmatrix}0 & E\\ E & 0\end{pmatrix},\ 0=\begin{pmatrix}0 & 0\\ 0 & 0\end{pmatrix},\ E=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}.$$

Therefore Hamiltonians remain invariant:

$$H'(x',t')=H(x,t).$$

The transformed Hamiltonian concerns, however, with the same process in the new coordinate system. Since in the inverse process events must occur in the order of increasing t' and so initial and final states and emission and absorption processes must interchange respectively with each other, the Hamiltonian of the inverse process is the transposed matrix of $H'(x',t')$, so the next relation holds:

$$(p_1'|H'(t)|p_2')=(p_2|H(t)|p_1). \tag{2}$$

The fundamental equations of Tomonaga Schwinger theory

$$i\hbar\frac{\partial\Phi(n,t)}{\partial t}=H(t)\,\Phi(n,t),$$

$$\left.\begin{aligned} i\hbar\frac{\partial S(t_1,t_2)}{\partial t_1}&=H(t_1)\,S(t_1,t_2),\\ -i\hbar\frac{\partial S(t_1,t_2)}{\partial t_2}&=S(t_1,t_2)\,H(t_2)\end{aligned}\right\} \tag{3}$$

allow the transformation

$$x' = -x,\ t' = -t,$$

$$H'(x', t') = H^*(x, t),\quad (* \text{ transposition})$$

$$\Phi'(n, t') = \bar{\Phi}(n, t), \tag{4}$$

$$S'(t_1, t_2') = S^*(t_2, t_1), \tag{5}$$

and after which the equations become

$$i\hbar \frac{\partial \Phi'(n, t')}{\partial t'} = H'(t')\,\Phi'(n, t'),$$

$$\left.\begin{aligned} i\hbar \frac{\partial S'(t_1', t_2')}{\partial t_1'} &= H'(t_1')\,S'(t_1', t_2'), \\ -i\hbar \frac{\partial S'(t_1', t_2')}{\partial t_2'} &= S'(t_1', t_2')\,H'(t_2'). \end{aligned}\right\}$$

The S-matrix of the inverse is

$$(p_1' | S'(t_1', t_n') | p_n')$$

$$= 1 + \sum_{n=1}^{\infty} \left(\frac{-ie}{\hbar c}\right)^n \int \Theta'(t_1', t_2', \ldots, t_n')$$

$$\cdot H'(t_1')\,H'(t_2') \ldots H'(t_n')\,dt_1'\,dt_2' \ldots dt_n', \tag{6}$$

where $\Theta'(t_1', t_2', \ldots, t_n')$ takes non zero value only when $t_n', \ldots, t_2', t_1'$ is monotonically increasing series. Since this condition is the same as that $t_1, t_2, \ldots, t_n$ is monotonically increasing series,

$$\Theta'(t_1', t_2', \ldots, t') = \Theta(t_n, \ldots, t_2, t_1). \tag{7}$$

Using the relations (2) and (7), we can put the expression (6) into the following form

$$1 + \sum_{n=1}^{\infty} \left(\frac{-ie}{\hbar c}\right)^n \int \Theta(t_n, \ldots, t_2, t_1)$$

$$H(t_n) \ldots H(t_2)\,H(t_1)\,dt_n \ldots dt_2\,dt_1,$$

which is the S matrix of the original process $(p_n | S(t_n, t_1) | p_1)$.
Thus we have the relation

$$(p_1' | S'(t_1', t_n') | p_n') = (p_n | S(t_n, t_1) | p_1). \tag{8}$$

This shows that the inverse process $p_n' \to p_1'$ occurs with the same probability as the original process $p_1 \to p_n$.

The above considerations are performed concerning (x, t) description, but the same are also possible concerning (x, σ) description, σ being any space like surface. By our inversion procedure any space like surface σ turns into corresponding space like surface σ' with the inversed configuration. We can make the same discussions as above made also with $H(x, \sigma)$ or $S(\sigma_1, \sigma_2)$ instead of $H(x, t)$ or $\sigma(t_1, t_2)$, without any alteration of physical results. Thus we can obtain the same physical result in the general form

$$(p'(\sigma_1') | S'(\sigma_1', \sigma_n') | p'(\sigma_n'))$$

$$= (p(\sigma_n) | S(\sigma_n, \sigma_1) | p(\sigma_1)),$$

which means the inverse process occurs with the same probability in the most general case.

2. Time inversion operator

Now let us investigate transformation properties of fields in the case of coordinate inversions. About tensor fields there is no question, so we will discuss only the case of spinor fields, and then, however, it may be sufficient to take up the fundamental case of Dirac electron field only.

The electron wave equation due to Dirac is

$$\{\gamma_\lambda p_\lambda + mc\}\,\Psi = 0 \tag{9}$$

where

$$p_l = -i\hbar \frac{\partial}{\partial x_l},\ p_4 = i\hbar \frac{\partial}{\partial x_4};$$

$$\lambda = 1,2,3,4\ ;\ l = 1,2,3,4, \tag{10.a}$$

$$(x_1, x_2, x_3, x_4) = (x, y, z, ct),$$

$$\gamma_l = \gamma_4 \rho_1 \sigma_l = \begin{pmatrix} 0 & \sigma_l' \\ -\sigma_l' & 0 \end{pmatrix},\quad \gamma_4 = \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}, \tag{10.b}$$

$$\rho_1 = \begin{pmatrix} 0 & E \\ E & 0 \end{pmatrix},\quad \sigma_l = \begin{pmatrix} \sigma_l' & 0 \\ 0 & \sigma_l' \end{pmatrix},$$

$$\sigma_1' = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma_2' = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \sigma_3' = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

$$E = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},\quad O = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \tag{10.c}$$

$$\Psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} = \begin{pmatrix} \psi \\ \varphi \end{pmatrix},\ \psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix},\ \varphi = \begin{pmatrix} \psi_3 \\ \psi_4 \end{pmatrix}. \tag{10.d}$$

For the coordinate inversion

$$(x_1, x_2, x_3, x_4) \to (\varepsilon_1 x_1,\ \varepsilon_2 x_2,\ \varepsilon_3 x_3,\ \varepsilon_4 x_4),$$

$$\varepsilon_\lambda = \pm 1, \tag{11}$$

the corresponding spinor transformation S can be obtained by solving four equations corresponding to (11)

$$S\gamma_1 S^{-1}=\varepsilon_1\gamma_1, \quad S\gamma_2 S^{-1}=\varepsilon_2\gamma_2,$$
$$S\gamma_3 S^{-1}=\varepsilon_3\gamma_3, \quad S\gamma_4=S^{-1}=\varepsilon_4\gamma_4. \qquad (12)$$

If S can be obtained and the wave function transforms according to S, the wave equation (9) remains invariant under the coordinate inversion (11). For several typical inversions, S's are obtained as follows.

(i) *plane reflection :* $T(-x_l, t)$,

for example, $T(-x_1 t)$ *concerning* $x_2 x_3$ *plane.*

$$(x_1,x_2,x_3,x_4)\rightarrow(-x_1,x_2,x_3,x_4),$$
$$S(-x_l,t)=\begin{pmatrix}\sigma_l' & 0\\ 0 & \sigma_l'\end{pmatrix}. \qquad (13.a)$$

(ii) *space inversion :* $T(-r, t)$,

$$(x_1, x_2, x_3, x_4)\rightarrow(-x_1, -x_2, -x_3, x_4),$$
$$S(-r, t)=\begin{pmatrix}E & 0\\ 0 & -E\end{pmatrix}. \qquad (13.b)$$

(iii) *time inversion :* $T(r,-t)$

$$(x_1, x_2, x_3, x_4)\rightarrow(x_1, x_2, x_3, -x_4),$$
$$S(r, -t)=\begin{pmatrix}0 & E\\ -E & 0\end{pmatrix}. \qquad (13.c)$$

(iiii) *space-time inversion :*

$$T(-r, -t),$$
$$(x_1, x_2, x_3, x_4)\rightarrow(-x_1, -x_2, -x_3, -x_4),$$
$$S(-r, -t)=\begin{pmatrix}0 & E\\ E & 0\end{pmatrix}. \qquad (13.d)$$

The wave equation (9) involves the spin operators $\sigma_1, \sigma_2, \sigma_3$. These operators have the proper values $+1$ and -1. If we denote the wave functions belonging to $+1$ or -1 values of σ_l spin with $\Psi_{\sigma l}{}^{+}$ or $\Psi_{\sigma l}{}^{-}$ respectively, they must have the following forms in order to be the proper functions of the matrix σ_l.

$$\Psi^{+}_{\sigma_1}=\begin{pmatrix}a\\ a\\ c\\ c\end{pmatrix}, \Psi^{-}_{\sigma_1}=\begin{pmatrix}a\\ -a\\ c\\ -c\end{pmatrix}, \Psi^{+}_{\sigma_2}=\begin{pmatrix}a\\ ia\\ c\\ ic\end{pmatrix},$$
$$\Psi^{-}_{\sigma_2}=\begin{pmatrix}a\\ -ia\\ c\\ -ic\end{pmatrix}, \Psi^{+}_{\sigma_3}=\begin{pmatrix}a\\ o\\ c\\ o\end{pmatrix}, \Psi^{-}_{\sigma_3}=\begin{pmatrix}o\\ b\\ o\\ d\end{pmatrix}. \qquad (14)$$

Under the coordinate inversions T's of (13) these wave functions undergo the transformation S's of (13) and the transformed functions remains to be in the state of the same spin value or turns into the state of the opposite sign spin value. We may denote these circumstances as $\sigma_l\rightarrow\sigma_l$ or $\sigma_l\rightarrow-\sigma_l$ respectively according to $\Psi_{\sigma l}{}^{\pm}\rightarrow\Psi_{\sigma l}{}'^{\pm}$ or $\Psi_{\sigma l}{}^{\pm}\rightarrow\pm\Psi_{\sigma l}{}'^{\mp}$. Thus we can investigate the behaviors of spins under coordinate inversions, and the obtained results can be summarized as follows.

(i) *plane reflection :* $T(-x_i,t)$ *concerning to* $x_j\ x_k$ *plane.*

$$\sigma_i\rightarrow\sigma_i, \quad \sigma_j\rightarrow-\sigma_j, \quad \sigma_k\rightarrow-\sigma_k. \qquad (15.a)$$

(ii) *space inversion :* $T(-r, t)$,

$$\sigma_l\rightarrow\sigma_l \qquad (15.b)$$

(iii) *time inversion :* $T(r,-t)$,

$$\sigma_l\rightarrow\sigma_l. \qquad (15.c)$$

(iiii) *space-time inversion:* $T(-r, -t)$,

$$\sigma_l\rightarrow\sigma_l. \qquad (15.d)$$

Thus we have seen that the spins remain invariant under the time inversion or space-time inversion, contrary to the old time-reversal operation of Wigner, used by F, Coester. Moreover also in the quantized theory circumstances hold equally, for Hamiltonians become the tranposed matrices and wave functions become the complex conjugate.

In conclusion, the author wishes to express his sincere thanks to Prof. K. Husimi for suggesting this investigation to him, and he is also deeply grateful to Dr. R. Utiyama for valuable discussions.

1) F. Coester, Phys. Rev. **84** (1951), 1259.
2) E. P. Wigner, Goettinger Nachr. (1932), 546.

Note on the Law of Conservation of Heavy Particles*

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Nambu *et al.* and the present author[1] proposed a theory which treats the V^0 as a *heavy nucleon*. Pais[2] attempted a classification of elementary particles and took seriously the conservation of nucleons. In a previous note[3], the author tried the ordering of the newly-found particles and gave attention to the *conservation of heavy particles*. It is the purpose of this note to express the idea mentioned there in a more clear form. No phenomenon has yet been observed without the formation of another heavy particle and, in particular, the proton appears to be entirely stable. As regards the stable particles, which never undergo natural decays, only two sorts of them are believed to be stable, that is, proton and the lightest group such as electron, neutrino, γ-ray and possibly μ^0-meson. This fact may be of interest, but the existence of other sorts of stable particles cannot be denyed in the present state of our knowledge. As unstable particle will ultimately disintegrate into lighter stable particles, there exists the ultimate interaction between this unstable particle and their stable decay products. So in every interaction scheme we can replace unstable particles by their ralated stable particles. By this procedure, all interactions containing unstable particles can be reduced to certain couplings between only stable particles. Of course, this reduction is not unique and there may be various types of couplings between stable particles. For guaranteeing sufficient[4] stability of matter we may postulate the following *ad hoc assumption*; "*In every possible interaction schemes between stable elementary particles, the difference of the number of protons and anti-protons should be conserved.*"

Eliminating intermediate unstable particles we can lead the following types of interactions between certain elementary particle A and stable particles.

$$A \rightleftarrows m\ proton + n\ anti\text{-}protons + other\ stable\ particles. \qquad (1)$$

Assign a characteristic number

$$\lambda = m - n \text{ to } A \text{ as } A(\lambda).$$

Consequence (I)

The assignment of λ-value to A is unique.

This is because otherwise by the intermediary of A, reaction will occur which is incompatible with the above *assumption*. By (1),

Consequence (II)

If the field $A(\lambda)$ has complex amplitude, the charge conjugate field A^c of $A(\lambda)$ has $-\lambda$. Real field has both signs of λ and canno have unique λ-value.

Consequence (III)

Neutral particles which have non-zero λ-values could not be described by real fields[5].

This is true for *neutron* and V^0[6].

Consequence (IV)

Those particles which are lighter than proton should have $\lambda=0$. Proof: For the stable particle lighter than proton, it is clear from (1) and our *assumption*. Unstable particle lighter than proton does not contain proton and anti-proton in their stable decay products, so it has $\lambda=0$. However, it does not follow that all particles heavier than proton should have $\lambda=0$. It means that among particles with $\lambda\neq 0$, *proton* is the lightest particle. Note also that the assignment of λ not relate a priori to the *spin* of that particle. Consider the general interaction $A^c(\lambda_a)B^c(\lambda_b)C^c(\lambda_c)\ldots L(\lambda_l)\ M(\lambda_m)\ N(\lambda_n)\ldots$ which is assumed to satisfy every conditions for elementary interaction.

Consequence (V)

This interaction could be allowd in only the cases when

$$-(\lambda_a+\lambda_b+\lambda_c+\ldots) + (\lambda_l+\lambda_m+\lambda_n+\ldots)=0.$$

This is the explicit expression of our postulate and may be compared with *the conservation of electric charge* in any reaction. Nucleon-photon interaction gives $\lambda=1$ for proton and neutron-decay and V^0-decay imply $\lambda=1$ for these particles. To our regret, the deeper cause for *the conservation law of heavy particles* is unknown. The characteristic number λ may be hoped to be attributed to some *intrinsic properties* of elementary particles. Indeed, Wigner's proposition[7] seems to interpret the conservation of λ as the conservation of, as it were, *neutronic* or *mesic charge*, and Tiomno and Yang[8] referred to this principle in their treatment of *reflection* properties of spin $\frac{1}{2}$ particle. The more comprehensive studies of the interactions between elementary particles will be published in the later issue of this journal. This work was completed during my stay in Nagoya University. The author wishes to express his thanks to Prof. Sakata and his collabora-

tors for their hospitality and uselul discussions. He is also indebted to Mr. Hori for his kind discussions.

*) Read at the Kyoto Meeting of the Physical Society of Japan, October 31, 1952.

1) Y. Nambu, K. Nishijima and Y. Yamaguchi, Prog. Theor. Phys. **6**(1951), 615, 619: S. Ôneda, Prog. Theor. Phys. **6** (1951), 663, 1014.
2) A. Pais, Phys. Rev. **86** (1952), 663.
3) S. Ôneda, Prog. Theor. Phys. **8**(1952), 255.
4) It may not be a necessary condition.
5) In this point the author owes much to the kind discussions of Nagoya group.
6) See references (1) and (2). Also L. I. Schiff, Phys. Rev. **85** (1952), 374.
7) E. P. Wigner, Proc. N. A. S. **38**(1952), 449, The author wishes to express his thanks to Prof. Tomonaga for noticing him Wigner's work.
8) J. Tiomno and C. N. Yang, Phys. Rev. **79**(1950), 495.

On the Convergence of the S-matrix Series

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Recently F. J. Dyson[1] has conjectured that the power series of the coupling constant e representing the renormalized S-matrix in q. e. d. (which we will call hereafter *S-matrix series*) may be divergent. However, contradiction seems to be present between the physical pictures and the mathematical definition of his fictitious world. Here we estimated its convergence property from *rather* mathematical stand-point.

In what follows, we are obliged to use some abbreviations for typographical reasons. We will avoid as far as possible to write vector or spinor indices explicitly. By coordinates in square brackets or braces, we will denote the corresponding suppressed indices together with them :

$$\rho_i, y_i = [y_i],\ \bar{u}_j, \bar{x}_j = \{\bar{x}_j\},\ u_k, x_k = \{x_k\}, \quad (1)$$

for example

$$A_{\rho(i)}(y_i) = A([y_i]),\ \bar{\psi}_{\alpha(j)}(x_j) = \bar{\psi}(\{x_j\}),$$
$$\psi_{\alpha(k)}(x_k) = \psi(\{x_k\}).$$

And if we must write them explicitly, we will express them as, for example,

$$(\gamma_\rho)_{\bar{\alpha}\alpha} = \gamma(\rho\,;\,\bar{\alpha}\alpha). \quad (2)$$

The convergence of the S-matrix can be ascribed to that of its element, hence of $\boldsymbol{A}$, if we write the S-matrix as,

$$S = \sum_{r=0}^{\infty}\sum_{s=0}^{\infty}\int d\bar{x}_1 dx_1 \cdots d\bar{x}_r dx_r dy_1 \cdots dy_s \times$$
$$\boldsymbol{A}(e\,;\,\{\bar{x}_1\}\{x_1\}\cdots\{\bar{x}_r\}\{x_r\}\,;\,[y_1]\cdots[y_s])$$
$$\cdot\bar{\psi}(\{\bar{x}_1\})\psi(\{x_1\})\cdots\times$$
$$\bar{\psi}(\{\bar{x}_r\})\psi(\{x_r\})A([y_1])\cdots A([y_s])\colon \quad (3)$$

The coefficient $\boldsymbol{A}$ has been calculated by S. Tomonaga and N. Fukuda[2] as a power series of e,

$$\boldsymbol{A} = (-1)^r \frac{e^s}{(r!)^2 s!}\sum_{n=0}^{\infty} e^{2n}\frac{[(2n+s)!]^2}{(2n+s-r)!\,2^n n!}\times$$
$$\int d\bar{x}_{r+1}dx_{r+1}\cdots d\bar{x}_{2n+s}\ dx_{2n+s}\times$$
$$S_F(\{x_{r+1}\}-\{\bar{x}_{r+1}\})\cdots$$
$$\cdots\cdots\cdots S_F(\{x_{2n+s}\}-\{\bar{x}_{2n+s}\})\times$$
$$\frac{1}{[(2n+s)!]^2}\sum_P\sum_{P'}\delta_P\delta_{P'}\{\gamma(\rho_1;\bar{u}_{i(1)}u_{j(1)})\cdots$$
$$\cdots\cdots\cdots\gamma(\rho_s;\bar{u}_{i(s)}u_{j(s)})\times$$
$$\gamma(\mu';\bar{u}_{i(s+1)}u_{j(s+1)})\ \gamma(\mu';u_{i(s+2)}u_{j(s+2)})\cdots$$
$$\gamma(\mu^{(n)};\bar{u}_{i(2n+s-1)}u_{j(2n+s-1)})\times$$
$$\gamma(\mu^{(n)};\bar{u}_{i(2n+s)}u_{j(2n+s)})\times$$
$$D_F(x_{j(s+1)}-x_{j(s+2)})D_F(x_{j(s+3)}-x_{j(s+4)})\cdots$$
$$\cdots\cdots\cdots D_F(x_{j(2n+s-1)}-x_{j(2n+s)})\times$$
$$\delta(\bar{x}_{i(1)}-x_{j(1)})\cdots\delta(\bar{x}_{i(2n+s)}-x_{j(2n+s)})\times$$
$$\delta(x_{j(1)}-y_1)\cdots\delta(x_{j(s)}-y_s)\}, \quad (4)$$

where δ_P, $\delta_{P'}$, are ± 1 according as permutations

$$P = \begin{pmatrix} 1, 2, \ldots\ldots, 2n+s \\ i(1), i(2), \ldots, i(2n+s) \end{pmatrix},$$

$$P'=\begin{pmatrix} 1, & 2, \ldots\ldots, & 2n+s \\ j(1), & j(2), \ldots, & j(2n+s) \end{pmatrix}$$

are even or odd. The equation (4) can be also obtained from the formula given by the author[3].

If we replace the values of $[(2n+s)!]^2$ integrals in the Eq. (4) by a mean value I_n, we have

$$\boldsymbol{A}=(-1)^r \frac{e^s}{(r!)^2 s!} \sum_{n=1}^{\infty} e^{2n} \frac{[(2n+s)!]^2}{(2n+s-r)!\,2^n n!} I_n. \tag{5}$$

The coefficient $[(2n+s)!]^2/(2n+s-r)!\,2^n n!$ increases as $2^n n!$. Therefore the series (5) does not fulfil the necessary condition of convergence, i.e. the n-th term$\to 0$, $(n\to\infty)$, unless a factor sufficiently small to compensate it appears from I_n. In reality, however, some of the $[(2n+s)!]^2$ integrals identically vanish corresponding to unnecessary Feynman graphs. At first, integrals with $i(m)=j(m)$ $(1\leqq m\leqq 2n+s)$ should vanish which would not appear if we have employed the antisymmetrized expression of the current operator. Thus the number of the integrals reduces to $[(2n+s)!]^2 \sum_{r=0}^{2n+s}(-1)^r(1/r!)$ which nearly equal to $[(2n+s)!]^2$ $(1/\varepsilon)$ for large n, where ε is the base of natural logarithmus $(\varepsilon=2.7\cdots)$. Second, there are contained in I_n, integrals corresponding to separate graphs and integrals to vanish according to Furry's theorem. If we omit, for estimation, every graphs with at least one loop, only I_n with $j(1)\ldots j(2n+s)$ obtained from $i(1)\ldots i(2n+s)$ by a cyclic permutation appear in the Eq. (5). Thus the number of integrals reduces by $1/(2n+s)$.

But in each case the coefficient of the n-th term increases infinitely with n. Therefore, it seems probable that the series (5) cannot be expected to converge, though we cannot assert until explicit calculation of I_n will be performed. The Eq. (5) with $r=2$, $s=0$ corresponds to the result of C. A. Hurst[4]. A weak point of this estimation is that we treated $\boldsymbol{A}$ ae if it had already been renormalized.

1) F. J. Dyson, Phys. Rev. **85**(1952), 631.
2) S. Tomonaga and N. Fukuda, Soryusiron Kenkyu (Mimeographed circular in Japanese) Vol. 3, No. 2 (1951), 1.
3) S. Hori, Prog. Theor. Phys. **7**(1952), 578.
4) C. A. Hurst, Phys. Rev. **85** (1952), 920.

Generalization of Analytical Spin

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November 24, 1952

In my previous letter[1] it was shown that the three components of the Pauli spin were represented as the analytical operators

$$\sigma_x=2\left(\cos\omega\frac{\partial}{\partial\chi}-\sin\omega\frac{\partial}{\partial\omega}\right),$$

$$\sigma_y=2\left(\sin\omega\frac{\partial}{\partial\chi}+\cos\omega\frac{\partial}{\partial\omega}\right), \tag{1}$$

$$\sigma_z=\frac{2}{i}\frac{\partial}{\partial\omega},$$

operating on the spin eigenfunctions

$$v_+=\exp[(\chi+i\omega)/2],$$
$$v_-=\exp[(\chi-i\omega)/2], \tag{2}$$

where χ and ω were independent variables.

Now the extension to the Dirac spin[2] is easily attained. Introducing one more variable φ, we get as the spin operators

$$\alpha_x=4\left(\cos\varphi\frac{\partial}{\partial\chi}-\sin\varphi\frac{\partial}{\partial\varphi}\right)\left(\cos\omega\frac{\partial}{\partial\chi}-\sin\omega\frac{\partial}{\partial\omega}\right),$$

$$\alpha_y=4\left(\cos\varphi\frac{\partial}{\partial\chi}-\sin\varphi\frac{\partial}{\partial\varphi}\right)\left(\sin\omega\frac{\partial}{\partial\chi}+\cos\omega\frac{\partial}{\partial\omega}\right), \tag{3}$$

$$\alpha_z=\frac{4}{i}\left(\cos\varphi\frac{\partial}{\partial\chi}-\sin\varphi\frac{\partial}{\partial\varphi}\right)\frac{\partial}{\partial\omega},$$

$$\beta=\frac{2}{i}\frac{\partial}{\partial\varphi},$$

and as the eigenfunctions

$$v_1=\exp[(\chi+i\varphi+i\omega)/2],$$

$$v_2=\exp[(\chi+i\varphi-i\omega)/2],$$
$$v_3=\exp[(\chi-i\varphi+i\omega)/2], \quad (4)$$
$$v_4=\exp[(\chi-i\varphi-i\omega)/2].$$

Since the eigenvalue of the square of each of (3) becomes unity and that of the anti-commutator of any two components vanishes, the eigenstates of the Dirac particle are represented as scalar functions of x, y, z, t and χ, φ, ω. For the free particle with positive energy and spin, for instance, we have

$$\psi=[(m+\sqrt{p^2+m^2})v_1+p_z v_3$$
$$+(p_x+ip_y)v_4]\cdot\exp[i(px-Et)]. \quad (5)$$

In a similar way, it is possible to represent the spin matrices with 2^n rows and columns analytically with $(n+1)$ independent variables $\omega_1, \omega_2, \ldots\omega_n$ and χ. Then the 2^n eigenfunctions are defined as follows

$$v=\exp[(\chi\pm i\omega_1\pm i\omega_2\ldots\pm i\omega_n)/2]. \quad (6)$$

1) T. Yamamoto, Prog. Theor. Phys. 8 (1952), 258(L).
2) P. A. M. Dirac, Proc. Roy. Soc. A117(1928), 610.

Propagation of the Cosmic Radiation through Intersteller Space

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November 25, 1952

The purpose of this short note is to present an additional evidence that the cosmic radiation passes through only a small thickness of intersteller matter. This has already been suggested through studies on primary heavy nuclei. Bradt and Peters[1] found in the primary cosmic radiation a negligible amount of Li, Be and B, which could be produced by the collisions of heavier nuclei with intersteller matter. Their passage is, therefore, limited within a few gcm^{-2} of matter. Dainton et al[2]. however, obtained an evidence which contradicts the former result. In spite of this discrepancy between above two experiments, the existence of heavy nuclei, such as C, O, Ne and Fe, may set the upper limit of about 10 g cm^{-2} to the amount of intersteller hydrogen traversed, as pointed out by Dainton et al[2]. provided the assumption of cosmic elements and the velocity spectra of nuclei at the origin are accepted.

This concept disagrees with the speculation of Fermi[3] and Unsöld[4], who assumed the cosmic radiation as confined in our galaxy due to the galactic magnetic field, avoiding a difficulty that the cosmic radiation takes up too great energy in the universe. According to these authors, the cosmic radiation possesses a mean life time in the galaxy, corresponding to the absorption mean free path in the matter. Then the mean free path for cosmic ray protons is the order of 100g cm^{-2}, which seems to be long enough to produce an appreciable amount of secondary rays. Most of them are unstable and turn eventually into electrons and photons. The photons escape the galaxy and give a very small intensity observed. The electrons are, however, stored in the galaxy due to the magnetic field and may be observable on the earth, if they could not be eliminated during their travel through the galaxy.

The intensity of the electrons relative to that of protons may be estimated in the following way. Most of the electrons should mainly come from the decay of muons which are the daughters of pions, At the geomagnetic latitude 55^0 N, where experiments referred are carried out, the minimum energy of electrons for vertical incidence is 1,7 Bev. An electron of this energy can be produced through the decay of a muon of average energy of 5 Bev, consequently of a pion of 6 Bev. The minimum energy of a proton that can produce a pion of this energy due to a collision with hydrogen is 10 Bev. Taking into account the recoil of nucleons and the production of neutral pions, we may safely set the minimum energy of a proton which can effectively produce an observable electron as 20 Bev. Thus about 5% of protons are responsible to observable electrons.

As seen above, we would expect an appreciable amount of electrons in the primary cosmic radiation, unless there were any efficient absorption process for the electrons. This problem has been studied by Donahue[5], asking whether or not the electrons originally accelerated together with nuclei could be eliminated during their passage through intersteller space. The result of this author can be applied to our case. The mean life time of electrons determined by the Compton scattering with galactic photons is estimated

as about 4×10^{15} sec for an electron of energy 10 Bev losing a half of its energy. This life time is longer than the collision mean time for protons, about 7×10^{14} sec, and the intensity of electrons must be multiplied by the ratio of these life times. Thus the electron intensity turns out to be about 30% of the proton intensity. (This figure gives only a crude order of magnitude due to our meager knowledge on the pion production at high energies and may allow an uncertainty of factor two.) This definitely contradicts the experimental evidence on the absence of primary electrons[6].

On account of the inefficiency of eliminating electrons in the galaxy, we are led to the conclusion that protons should not travel in the galaxy for such long time as to produce electrons more than 0.6% of the total intensity. This set the upper limit of the path length for protons that they must not traverse more than 3 g cm^{-2} of hydrogen.

This evidence together with those mentioned above on heavy nuclei leads us to the presumption that the cosmic radiation passes through a very small amount of matter from its origin to entry. We are then inclined to reject the assumption that the cosmic radiation is confined in our galaxy for long time, but to adopt that it originates somewhere out of our galaxy and travels along a straight way. In this case one expects the siderial time variation of heavy primaries, because the earth locates far from the center of the galaxy and the amount of hydrogen traversed by the cosmic radiation coming through the center is about 0.6g cm^{-2}. In the passage through this thickness secondary particles are scarcely produced except photons which are due to the decay of neutral pions. The intensity of the secondary photons are estimated as about 0.1% of the total intensity at the geomagnetic latitude 55°, but as nearly 1.5% at the equator. In the latter case this effect would be detectable.

Full account will be published in the Journal of Geomagnetism and Geoelectricity, Japan.

1) H. L. Bradt and B. Peters, Phys. Rev. **77** (1950), 54; **80** (1950), 943.
2) A. D. Dainton, P.H. Fowler and D.W. Kent, Phil. Mag. **42** (1951), 317; **43** (1952), 729.
3) E. Fermi, Phys. Rev. **75** (1951), 1169.
4) A. Unsöld, Phys. Rev. **82** (1951), 857.
5) T. M. Donahue, Phys. Rev. **84** (1951), 972.
6) C.L. Critchfield, E. P. Ney and S. Oleska, Phys. Rev. **85** (1952), 461.

On the Corpuscular Aspect of Quantum Theory of Field

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The relativistic problem of bound systems has been recently treated by several authors[1]. Common characteristics of these works are the appearance of the wave functions and the kernels or the Green functions which are the functions of coordinates of particles. However, the physical meaning of these quantities is not so obvious in their works.

The wave function of ordinary wave mechanics is interpreted as the probability amplitude. It is, therefore, interesting to investigate how to define the wave functions which admit such a primitive physical interpretation in the frame of present field theories.**)

In quantum field theories which admit creation and annihilation of particles, the number of particles is not generally conserved, so it is natural to expect the damping properties of the wave function with fixed number of particles. From this point of view, Gell-Mann and Low's work seems to be a little contradictory, which has, in fact, the following inconsistencies: (i) In spite of the stationary property of the wave function χ_n by its definition, the equation of χ_n derived by the "L-operation" seems to have generally damping solutions. (ii) The equation of χ_n derived directly from the definition does not coincide with the equation obtained by the "L-operation". The correspondence of true stationary states and free stationary states through the adiabatic switch-on process is not necessarily one to one. Then it is not always possible to obtain the equation of single χ_n by the "L-operation".

For simplicity we shall discuss the one-particle problem of quantum electrodynamics. In order to obtain the reasonable definition of the wave function, we should express the state that a physical electron exists at a point x and time t. We may take $\psi_H^*(x,t)\Psi_0$ for this state because of following reasons: (i) This is the eigenstate belonging to the eigenvalue $-e$ of the total charge operator. (ii) The expectation value of charge density operator at time t is independent of t, and is a function of the distance from x, concentrating in the neighborhood of the point x with the extension of order of magnitude

of Compton wave length. (iii) This state takes into account of the effect of surrounding electromagnetic field.

The concept of the position of electron has only a diffused meaning (see above (iii)), while the state $\psi_H^*(\boldsymbol{p},t)\Psi_0$ represents a physical electron with sharp momentum $\boldsymbol{p}$. Such a situation is characteristic of the relativistic quantum mechanics.[2)]

Now we consider the operators in field theories having the following properties:

$$[\psi_H(x,t), O_H(t)] = D\psi_H(x,t),$$

$$O_H(t)\Psi_0 = O_0\Psi_0$$

where D is a c-number operator operating on spinor indices or coordinates and O_0 is a c number. These conditions are satisfied by the many physically significant operators. For such a operator, the matrix element between the states of the distributions $f(x)$ at time t' and $g(x)$ at time t becomes

$$<g,t|\,O(t) - O_0|f,t'> = \int g^*(x)\,D\chi(xt)\,d^3x$$

where

$$\chi(x,t) = \frac{1}{i}\int_{t>t'} G(x,t;x',t')\,\beta f(x')\,d^3x'.$$

Here G is Schwinger's Green function. Thus we can reasonably take $\chi(x,t)$ as the one-electron wave function, which satisfies the equation given by Schwinger.

The probability amplitude of transition to the distribution $g(x)$ at time t from $f(x)$ at time t' is given by

$$\int g^*(x)\,\chi(x,t)\,d^3x.$$

Hence the wave function $\chi(x,t)$ is the amplitude of transition to point x from $f(x')$. So, it may be reasonable to impose the ordinary boundary condition on χ. The expectation value of the above operator becomes

$$\int \chi^*(x,t)\,D\chi(x,t)\,d^3x.$$

In particular, the expectation value of the total energy operator takes generally a complex value. If we can obtain the energy value ss a solution of eigenvalue problem for the equation of χ. it is easily shown that its imaginary part gives the real decay constant.

The detailed report will be published in near future in this journal.

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**) Historically the quantum theory of field was first appeared as the second quantization. In this non-relativistic case, the corpuscular aspect is evident as shown by Fock in his well known paper.

***) $\psi_H(x,t)$ and Ψ_0 denote the spinor operator of electron and true vaccum state in Heisenberg representation, respectively.

1) E. E. Salpeter and H. A. Bethe, Phys. Rev. **84** (1951), 1232.
H. Kita, Prog. Theor. Phys. **7** (1952), 217.
M. Gell-Mann and F. Low, Phys. Rev. **84** (1951), 350.
J. Schwinger, Proc. N. A. S. **37** (1951), 452.

2) W. Pauli, *Hb. d. Phys. XXIV/1* p. 214.

π-D Scattering and Strong Coupling Theory

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Recent experiments on the scattering of π-mesons by deuterium and by hydrogen[1)2)] have revealed the facts that the cross sections for π-D scattering are smaller than the sum of those for π^+-H and π^--H, and that this difference becomes more remarkable as the energies of the incident mesons increase. It is a well-known fact that these effects are evidently in disagreement with the calculations based on the weak coupling theories or the impulse approximation. We shall briefly point out in this letter that the strong coupling theory can give a satisfactory account of these experimental facts.

We treat the interaction of free mesons with nucleons (or their isobars) as a perturbation,[3)] and a usual second order perturbation leads to formulae for the transition matrix elements (in the unit system $\hbar = c =$ meson mass $= 1$).

$$H_{fi}^I = \sum_j \frac{1}{\{\omega + (q^2/M + V)\}} \times$$

$$\times \frac{(f|H|j)\ (j|H|i)}{-\{E+k^2/4M+(q^2/M+V)_j\}}$$

and

$$H^{II}_{fi}=\sum_{j'}\frac{1}{\{\omega+(q^2/M+V)_i\}}$$

$$\times \frac{(f|H|j')\,(j'|H|i)}{-\{2\omega+k^2/4M+(q^2/M+V)_{j'}+E\}}.$$

Where H is the interaction Hamiltonian of free mesons with nucleons or their isobars, V is the potential between two nucleons (or their isobars) that constitute the deuteron, M is the mass of nucleons, q their relative momentum, ω and k the energy and momentum of the incident meson respectively, and E is the energy of the isobar with spin 3/2 which is taken to be 250Mev with imaginary part (half width) of~30Mev. f,i,j, and j' mean the final state, initial state, intermediate states in which the incident meson has been absorbed and no meson is present, and intermediate states in which the outgoing meson has been emitted and two mesons (incident and outgoing) are present, respectively.

Expanding these formulae with respect to V, and retaining the terms containing lower powers of V than linear only, we have

$$H^{I}_{fi}=\sum_{j}\frac{(f|H|j)\,(j|H|i)}{\omega-E-k^2/2M}$$

$$-\sum_{j}\frac{(f|H|j)\,(j|[H,V]|i)}{(\omega-E-k^2/2M)^2}$$

and a similar equation for H^{II}. These are just the expansion of Ashkin and Wick. The existence of isobars of nucleons makes the denominator of the second term small when the energy of the incident meson is near the isobar energy, and the second term (containing V) assumes a remarkably large value in contrast with the formulae deduced from weak coupling theories.

According to the pseudoscalar charge-symmetric meson theory of nuclear forces, V must be of the form[5]

$$V=\sum_{\alpha}(e^{\alpha}_{I}\ e^{\alpha}_{II})f(r)+\text{tensor force.}$$

For simplicity of calculations and because of its little contribution to the effect considered here, we neglect the effect of tensor forces. As our intermediate states consist of two nucleons with spin $S_1=1/2$ and $S_{II}=3/2$, the total spin S must be 1 or 2. The expectation values of $(e_I{}^{\alpha}e_{II}{}^{\alpha})$ are 5/9 for the states $S=1$, $-1/3$ for the states $S=2$ and $-1/3$ for the ground state of the deuteron. Therefore the matrix elements of the commutator $(j|[H,V]|i)$ assume non-vanishing value for intermediate states of $S=1$.

After remarking these, the matrix elements of H^{I} and H^{II} can easily be evaluated, and the cross sections of $\pi^{\pm}$-D and π^{+}-H plus π^{-}-H can be calculated from these matrix elements as plotted in the figure. We have here taken $f(r)$ as Hulthen's function with a scattering length fitted to the n-p scattering experimental data, and determined the magnitude of the potential so as to give a correct value for the binding energy of the deuteron. The interference effects are neglected throughout our calculations. The ratio

$$\{\sigma_H(\pi^+)+\sigma_H(\pi^-)-\sigma_D(\pi^{\pm})\}/$$
$$\{\sigma_H(\pi^+)+\sigma_H(\pi^-)\}$$

is 12 percent for the kinetic energy of incident mesons of 28Mev, while 25 percent for that of 112 Mev. Detailed accounts will be published in a later issue of this journal.

1) Isaacs, Sachs, and Steinberger, Phys. Rev. **85** (1952), 803.
2) Anderson, Fermi, Nagle and Yodh, Phys. Rev. **86** (1952), 413.
3) See Pauli and Dancoff, Phys. Rev. **62** (1942), 85.
4) Ashkin and Wick, Phys. Rev. **85** (1952) 686; see also Chew and Wick, Phys. Rev. **85** (1952), 636 and Chew and Goldberger, Phys. Rev. **87** (1952), 778.
5) Pauli and Kusaka, Phys. Rev. **63** (1943), 400.

A Note on the Gauge Transformation in the Theory of Non-local Interaction of the Fields

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Recently, Møller and Kristensen[1] have pointed out that one can construct the theory of fields free

from the difficulty of divergence, by taking as the Lagrangian for the interaction

$$L=f\int dxdx'dx''F(x,x',x'')\,U^{+}(x)\,l^{-}(x')U(x''), \quad (1)$$

provided that the form factor $F(x,x',x'')$ should be taken properly. In such a case, it is well known that the free fields itself need not be non-local.

Here we investigate whether we can keep the theory gauge invariant or not, when applied to the system of charged Fermions interacting with electromagnetic field.

We take the Lagrangian $\bar{L}$ for the interaction between electron and electromagnetic fields as follows

$$\bar{L}=-\hbar c\int\bar{\psi}(x)\left\{\gamma_\mu\frac{\partial\psi(x)}{\partial x_\mu}+\varkappa\psi(x)\right\}dx$$

$$-ie\iiint\bar{\psi}(x)\gamma_\mu\psi(x')\,A_\mu(x'')\times F(x,x',x'')\,dxdx'\,dx''. \quad (2)$$

Here $\psi(x)$, $A_\mu(x)$ denote Dirac spinor, electromagnetic 4-vector respectively.

We may define the gauge transformation as

$$A_\mu(x)\to A_\mu(x)+\frac{\partial\Lambda(x)}{\partial x_\mu},$$

$$\psi(x)\to\psi(x)\ \exp\left[\frac{ie}{\hbar c}\alpha(x)\right], \quad (3)$$

$$\alpha^*(x)=\alpha(x).$$

It is our interest to find a form of the function $\alpha(x)$ which keeps the interaction Lagrangian $\bar{L}$ invariant, under the above transformation. If $\alpha(x)$ depends on $\psi(x)$ and $\bar{\psi}(x)$, their commutation law

$$\{\psi(x),\ \bar{\psi}(x')\}=-iS(x-x'), \quad (4)$$

where

$$\{A,\ B\}=AB+BA,$$

cannot be gauge invariant. Hence $\alpha(x)$ must be independent of $\psi(x)$ and $\bar{\psi}(x)$.

We get easily the gauge transform $\bar{L}'$ of $\bar{L}$ as follows;

$$\bar{L}'=\bar{L}-ie\int dx\bar{\psi}(x)\left[\gamma_\mu\psi(x)\frac{\partial\alpha(x)}{\partial x_\mu}\right.$$

$$+\iint\gamma_\mu\psi(x')\left\{A_\mu(x'')\left(\exp\left[\frac{ie}{\hbar c}(\alpha(x')-\alpha(x))\right]-1\right)\right.$$

$$\left.\left.+\frac{\partial\Lambda(x'')}{\partial x_\mu''}\exp\left[\frac{ie}{\hbar c}(\alpha(x')-\alpha(x))\right]\right\}F(x,x',x'')dx'dx''\right]. \quad (5)$$

In order that $\bar{L}'=\bar{L}$, $\alpha(x)$ must satisfy the following equation;

$$\gamma_\mu\psi(x)\frac{\partial\alpha(x)}{\partial x_\mu}$$

$$+\iint\gamma_\mu\psi(x')\left\{A_\mu(x'')\left(\exp\left[\frac{ie}{\hbar c}(\alpha(x')-\alpha(x))\right]-1\right)\right.$$

$$\left.+\frac{\partial\Lambda(x'')}{\partial x_\mu''}\exp\left[\frac{ie}{\hbar c}(\alpha(x')-\alpha(x))\right]\right\}F(x,x',x'')dx'dx''=0, \quad (6)$$

$\alpha(x)$ is independent of $\psi(x)$ only when

$$F(x,x',x'')=G(x,x'')\delta(x-x'), \quad (7)$$

as the first term of Eq. (6) is a function of one point only. Then Eq. (6) reduces to

$$\frac{\partial\alpha(x)}{\partial x_\mu}=-\int\frac{\partial\Lambda(x'')}{\partial x_\mu''}G(x,x'')dx'' \quad (8)$$

and we can get $\alpha(x)$ independent of $\psi(x)$ only when

$$G(x,x'')=G(x\pm x''). \quad (9)$$

But, if $F(x,x',x'')$ does not have the form given by Eq. (7), $\alpha(x)$ must satisfy the following equation in order that Eq. (6) may hold for an arbitrary $\psi(x)$:

$$\frac{\partial\alpha(x)}{\partial x_\mu}\delta(x-x')=-\int\left\{A_\mu(x'')\left(\exp\left[\frac{ie}{\hbar c}(\alpha(x')-\alpha(x))\right]-1\right)\right.$$

$$\left.+\frac{\partial\Lambda(x'')}{\partial x_\mu''}\exp\left[\frac{ie}{\hbar c}(\alpha(x')-\alpha(x))\right]\right\}$$

$$F(x,x',x'')\,dx''. \qquad (10)$$

Here we used the formal relation

$$\gamma_\mu\psi(x)\frac{\partial a(x)}{\partial x_\mu}=\int\gamma_\mu\psi(x')\frac{\partial a(x)}{\partial x_\mu}\,\delta(x-x')\,dx'.$$

Now Eq. (10) is inconsistent as the left-hand side is a function defined at one point only and the right-hand side is not. Hence we cannot get $a(x)$ which satisfies Eq. (10); in other words, we cannot keep L gauge invariant. This means that Møller's theory of fields with the non-local interaction is not gauge invariant so long as the free fields are local.

Thus we are suggested that it may perhaps be necessary to use the non-local free fields interacting with each other, in order to keep the theory gauge invariant. Such a consideration is now in progress.

1) Møller and Kristensen, kgl. Danske. Vid. Sel. **27** (1952), No. 7.

Note on the Tensor Interaction in Triplet Odd States

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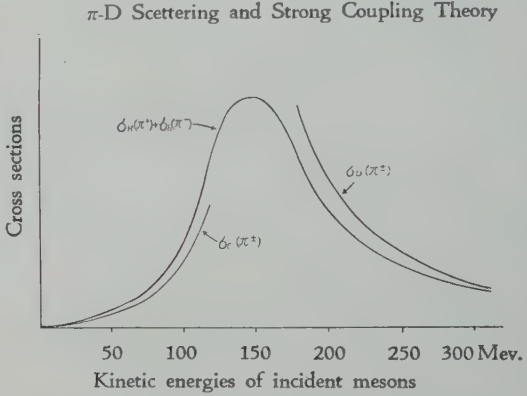
To explain the experimental angular distribution of proton-proton scattering at high energies, within the framework of the potential picture, singular tensor interaction has been proposed by Christian and Noyes[1] in triplet odd states. In these states central potentials are conclusively excluded, since in this case the scattering is zero at 90° and the angular cross section rises even more rapidly on either side of 90° than that shown by experiment. One can not, however, determine the sign of this tensor interaction definitely from high energy proton-proton scattering only.

On the other hand, Jastrow[2] has shown that it is possible to account for the n-p scattering data fairly good assuming a charge-independent interaction between nucleons. As that of Christian and Noyes, Jastrow's potential has a tensor interaction in triplet odd states, and its sign is completely determined as its magnitude. That is to say, the tensor force exchange dependence found necessary to explain high energy n-p scattering and deuteron quadrupole moment simultaneously is of the form $-V_0\ (1-a+aP_x)\ S_{12}$ with $a=0.6\sim0.7$ Therefore the effective potential in ${}^3P_1$ state is repulsive while the other two (${}^3P_0$ and ${}^3P_2$) are attractive.

Recently, very accurate measurements on proton-proton scattering at lower energies (1~4 Mev) have been done at Wisconsin University[3]. According to the results of phase shift analysis of these experiments, effective P-wave phase shifts are definitely negative, for example, $-0.074°\pm0.023°$ at 4.2 Mev showing the repulsive character of the effective potential in ${}^3P$ state as a whole.

Using these results, one can determine the sign of tensor interaction in triplet odd states and check the validity of the charge independent nuclear potential (namely Jastrow's potential). The presence of tensor interaction in ${}^3P$ state complicates the analysis of the scattering data[4] and exact treatment is very tedious. However, Breit[5] has pointed out that to the extent



that one can restrict oneself to the terms linear in the P-wave phase shifts, these enter only in the combination

$$K_1=\frac{1}{9}K({}^3P_0)+\frac{3}{9}K({}^3P_1)+\frac{5}{9}K({}^3P_2).$$

The resultant phase shift K_1 enters the scattering cross section in the same way as if no tensor force existed[6] and we can compare this value directly with that derived from experiment. We adopt this approximation and neglect the interaction between ${}^3P_2$-state and ${}^3F_2$-state which is of little importance at the

lower energies. Exact numerical integration of the wave equation is necessary since the resultant phase shift is zero K_1 identically in Born approximation.

Numerical calculations made for the case of Jastrow's potential gave values of $K(^3P_0)$, $K(^3P_1)$, $K(^3P_2)$ and resultant K_1 as in Table I.

Table I. Values of P-wave phase shift in degrees. Incident proton energy is 4.2 Mev. in the laboratory system.

$K(^3P_2)$	$K(^3P_1)$	$K(^3P_0)$	K_1
+0.133	−0.577	+1.832	+0.0852

Three P-wave phase shifts are small enough numerically so that the linear approximation adopted here will be valid. Resultant phase shift for Jastrow's potential has a wrong sign and can not explain above stated experiment.

From these result, we may conclude that if the resultant P-wave phase shift is negative as the experiments on proton-proton scattering at low energies show, the tensor interaction must have a different exchange dependence from that of Jastrow's potential and therefore it is impossible, by means of charge independent static potential, to account for the all experiments consistently.

More detailed calculation for this problem is in progress.

1) R. S. Christian and H. P. Noyes, Phys. Rev. **79** (1950), 85.
2) R. Jastrow, Phys. Rev. **81** (1951), 165.
3) J. N. Mc Gruer, D. E. Findley, and H. R. Worthington, Bullet. Americ. Phys. Soc. **27** (1952), 47.
Private communication from H. R. Worthington.
4) G. Breit, C. Kittel, and H. M. Thaxton, Phys. Rev. **57** (1940), 255.
5) G. Breit, University of Pennsylvania Bicentennial Conference, "*Nuclear Physics*" (1941), p. 10.
6) J. D. Jackson and J. M. Blatt, Rev. Mod. Phys. **22** (1950), 77.

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On the Structure of the Interactions of the Elementary Particles, III

—— *On the Renormalizable Field Theory* ——

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Some remarks are given on the renormalizable field theory. In § 1 the renormalizable field theory is defined as an assembly of spin 0 and $\frac{1}{2}$ fields and neutral vector fields (including the electromagnetic field) interacting each other via interactions of 1st kind only. In § 2 it is shown that there are several rules of renormalization, which lead to not necessarily identical finite results and remarks are given on the separation of divergences. In § 3 the outline of the renormalization method is given and there one can see the equivalence of the "subtraction" method and the "renormalization" method. In § 4 the gauge invariancy of the renormalized theory is examined and in the last section some comments are given on the present form of the theory.

§ 1. Renormalizable field theory

The interactions between the elementary particles in the present quantum field theory are usually assumed from the point of view of general requirements, e.g., relativistic covariancy, gauge invariancy, etc., which seem, however, to comprise much more theoretical possibilities than are realized in the nature. Recently, in the investigation of the problem of the renormalizability[1] the interactions have been classified into two distinct groups, that is, the interactions of 1st kind and those of 2nd kind. The renormalization theory, when applied to the former case, which is called hereafter the "renormalizable field theory", leads to a closed non-singular theory by introducing a finite number of counter terms, which also belong to the first kind. On the other hand, the existence of interactions of 2nd kind prevents the renormalization procedure from its closure. As to the existence of interactions of 2nd kind in the nature, the detailed account has been given in our previous paper[2]. Although the correct formulation is unknown for the case of interactions of 2nd kind,* it seems for us that the various difficulties appearing in this case, which are to be analysed in much more detail, are intimately connected with the problem of the structure of the elementary particles[1)2)].

In the present paper the general renormalizable field theory is investigated. In this theory, the following fields are accepted as having physical reality**:

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* A method of treating the interactions of 2nd kind will be developed in our following paper.

** The fields having spin $S \geqq 1$ and vanishing mass or those having spin $S=2$ or $3/2$ and interacting via two-vertex interactions only can belong to the renormalizable field theory. But, they are here excluded for lack of physical meaning. In this connection see also reference 2.

$$\left.\begin{aligned}&\text{charged and neutral fields with spin } 0,\ \phi^i(i=1,\ 2\cdots),\\&\text{charged and neutral fields with spin } \tfrac{1}{2},\ \psi^\alpha(\alpha=1,2\cdots),\\&\text{electromagnetic field, } A_\mu^0,\\&\text{neutral vector fields, } U_\mu^a(\text{mass}\neq 0)\ \ (a=1,\ 2\cdots).\end{aligned}\right\} \tag{1}$$

The vector couplings of U_μ^a-fields with ϕ^i- or ψ^α- fields*) belong to the interactions of the first kind. For, by use of the Stueckelberg formalism, we can in fact construct an unitary transformation, which results in the elimination of the B^a-component from the vector coupling interaction in the Schrödinger equation as follows[2]:

$$\left.\begin{aligned}&\left\{\frac{1}{i}\frac{\delta}{\delta\sigma(x)}-j_\mu^a A_\mu^a-\frac{1}{2}j_{\mu\nu}^a A_\mu^a A_\nu^a+H'\right\}\Psi(\sigma)=0,\\&U_\mu^a=A_\mu^a+\frac{1}{\varkappa_a}\partial_\mu B^a,\qquad (a=1,\ 2,\ 3\cdots)\end{aligned}\right\} \tag{2}$$

where H' is the sum of interactions other than the vector coupling of U_μ^a-field and j_μ^a and $j_{\mu\nu}^a$ involve neither A_μ^a nor B^a. The subsidiary condition becomes

$$\{\partial_\mu A_\mu^a+\varkappa_a B^a-\int_\sigma j_\mu^a(x')\Delta(x-x')d\sigma_\mu'\}\Psi(\sigma)=0. \tag{3}$$

The Schrödinger equation (2) has just the same form as in the case of the electromagnetic vector coupling, and so we can obtain the S-matrix of the same form in both cases. Only one difference between them lies in the invariant delta function, which are $\Delta(x)$ and $D(x)$ $((\Box-\varkappa^2)\Delta=0,\ \Box D=0)$ for the A_μ^a- part of U_μ^a- field and the electromagnetic field A_μ^0, respectively. The detailed discussion regarding this point will be given in the Appendix I (See also reference 2). Moreover, the theory of the neutral vector field is invariant under the following gauge-transformation:

$$\left.\begin{aligned}&A_\mu^a\to A_\mu^a+\partial_\mu\Lambda^a,\quad B^a\to B^a-\varkappa_a\Lambda^a,\\&(\Box-\varkappa_a^2)\Lambda^a=0.\end{aligned}\right\} \tag{4}$$

This transformation for A_μ^a is again of the same form as in the electromagnetic field A_μ^0. Thus, as proved in the Appendix I, we can obtain the electromagnetic field from the neutral vector field in the limit of $\varkappa_a\to 0$. From this fact it is allowed to denote hereafter the field quantities throughout both cases by the same notations $A_\mu^a(a=0$ implies the electromagnetic field and $a=1,\ 2,\ 3,\cdots$ other neutral vector fields).

The gauge transformation for the total system may now become

$$\left.\begin{aligned}&A_\mu^a\to A_\mu^a+\partial_\mu\Lambda^a,\\&\phi\to\phi^i e^{i\Lambda^i},\quad \psi^\alpha\to\psi^\alpha e^{i\Lambda^\alpha},\end{aligned}\right\} \tag{5}$$

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* The vector couplings are to be understood as the interaction between the source fields and the neutral vector field which is obtained by replacing the operator ∂_μ in the free Lagrangian by $\partial_\mu\pm ie_a U_\mu^a$.

$$\left.\begin{aligned} &\Lambda^i=\sum_a e_a^i \Lambda_a, \quad \Lambda^\alpha=\sum_a e_a^\alpha \Lambda_a, \\ &(\Box-\varkappa_a^2)\Lambda_a=0, \end{aligned}\right\}$$

where e_a^i's (or e_a^α's) are the coupling constants of the vector interactions between A_μ^a-field and ϕ^i-(or ψ^α-) fields and in particular e_0^i's (or e_0^α's) are the electric charges of charged i (or α) fields*).

As the interactions of the 1st kind consisting of A_μ^a-fields, we have $(A_\mu^a+1/\varkappa_a\cdot\partial_\mu B^a)\times(A_\mu^b+1/\varkappa_b\cdot\partial_\mu B^b)$, $F_{\mu\nu}^a F_{\mu\nu}^b (F_{\mu\nu}^a=\partial_\mu A_\nu^a-\partial_\nu A_\mu^a)$ and the above mentioned vector couplings. But, the primary interactions, which have not contained the term $(A_\mu^a+1/\varkappa_a\cdot\partial_\mu B^a)\times(A_\mu^b+1/\varkappa_b\cdot\partial_\mu B^b)$, do not require the introduction of interactions of this form as the counter terms of renormalization, because in this case B's are absent in the Schrödinger equation (2) and the terms $A_\mu^a A_\mu^b$ can not appear separately for the familiar reason of invariancy of the theory for the gauge transformation (5). Thus, the interactions of the form $(A_\mu^a+1/\varkappa_a\cdot\partial_\mu B^a)(A_\mu^b+1/\varkappa_b\cdot\partial_\mu B^b)$ are left out of consideration.

Thus, in our general discussion of renormalizable field theory we have only to consider the following interactions:

$$\left.\begin{aligned} &f_{ij}\phi^i\phi^j,\quad f_{ijk}\phi^i\phi^j\phi^k,\quad f_{ijkl}\phi^i\phi^j\phi^k\phi^l,\quad f_{\alpha\beta}\bar{\psi}^\alpha\psi^\beta,\quad f_{\alpha\beta i}\bar{\psi}^\alpha 0\psi^\beta\phi^i, \\ &\lambda_{ij}\partial_\mu\phi^{i*}\partial_\mu\phi^j, \\ &i(\delta_{ij}+\lambda_{ij})A_\mu^a(e_a^i\phi^{i*}\partial_\mu\phi^j-e_a^j\partial_\mu\phi^{i*}\phi^j)-(\delta_{ij}+\lambda_{ij})e_a^i e_b^j A_\mu^a A_\mu^b\phi^{i*}\phi^j, \\ &\lambda_{\alpha\beta}\bar{\psi}^\alpha\gamma_\mu\partial_\mu\psi^\beta,\quad -i(\delta_{\alpha\beta}+\lambda_{\alpha\beta})A_\mu^a e_a^\beta\bar{\psi}^\alpha\gamma_\mu\psi^\beta,\quad g_{ab}F_{\mu\nu}^a F_{\mu\nu}^b. \\ &\text{and their comp. conj.}\quad (0=1,\gamma^5\text{ etc.}). \end{aligned}\right\}\quad (6)^{**)}_{***)}$$

Some of these interactions, however, are excluded on accout of the requirements of the relativistic covariancy or charge conservation. For example, the interaction $\lambda_{ijk}\phi^i\phi^j\phi^k$ can not appear for the pseudo-scalar ϕ^i and scalar ϕ^j and ϕ^k. For the pseudo-spinor fields ψ^α the γ-matrices are to be suitably adjusted.

It was shown in the previous paper[1] that in the theory having the interactions of 1st kind only the resulting divergences in the S-matrix can always be brought into the form of interactions of 1st kind. Therefore, if we assume at the outset all the permissible interactions in the original Hamiltonian, then each diverging term will be always subtracted by any of the corresponding (counter) terms or the divergence will be renormalized into any of the coupling constants of them. The coupling constants of interactions (6)

* There may be the complex fields ϕ^i, ψ^α having no electromagnetic interaction, for which we take $e_0{}^i=e_0{}^\alpha=0$. In the following, the fields with non vanishing $e_a{}^i$ or $e_a{}^\alpha$ may be called "e_a charged" fields.

** The terms in (6) are the interaction Lagrangians. We can treat them, however, as the interaction Hamiltonians if the P- brackets are replaced by the Green functions everywhere. (See reference 10). In particular we shall give in the Appendix II the detailed discussions regarding the gauge invariant vector interaction of ϕ and ψ with $A_\mu{}^a$ (the 2nd to 4th lines of (6)).

*** Rigorously speaking, terms such as $f_i\phi^i$ are further to be added to (6), the contributions of which can be removed, however, by employing special evaluation rule of S-matrix.

or their renormalized values have to be determined by referring to the experimental results.

In this paper, some remarks on the general renormalizable theory are given. In § 2 it is investigated whether the finite result obtained from the theory are unique or not. In the renormalization theory some arbitrariness arises in connection with the treatment of the so-called overlapping divergences. Though the well-defined rule for treating them can give unique results it is possible that the different rules often give the different results. The best rule can never be singled out by the renormalization theory itself, but it must be selected through the consideration of experimental facts.

In § 3, the outline of the renormalization procedure is given. The treatment of divergences of two-vertex parts are considered in detail, which are one of the peculiar features in this theory. Further, we see there the equivalence between the usual two renormalization methods, that is, the method of the "self consistent subtraction"[1] and Dyson's method[3] of coupling constant renormalizations.

Since the observable charge is not the mechanical one, but the renormalized one, it is required that the renormalized theory is also invariant under the new gauge transformation or in other words, the counter terms, which have been separately determined so as to cancel the individual divergences, are gauge invariant as a whole (just as in (6)). In § 4 it is proved that this is the case provided that special attentions are paid to separating various divergent terms.

In the last sections some considerations are made in connection with the convergence of the perturbation series and the renormalized (actually diverging) coupling constants.

§ 2. Some remarks on renormalization rules

It can be shown that the renormalization theory, when applied to a system of fields with the interactions (6), gives finite results for the S-matrix elements.

When carrying through this procedure, special attentions must be paid, however, to the treatment of the so-called overlapping divergences, which are expected to occur in very complicated forms in our general case and from which there arise many ambiguities when removing the internal divergences. As to this point two methods have been presented by Salam[4] and Ward[5]. In this section we shall show that these two methods do not in general lead to the same result.

It is also shown below that in connection with the separation of divergences from the special type of non-overlapping graphs there appear ambiguities which are peculiar to our general case. It is also quite arbitrary how to treat them. Accordingly, we can establish the several possible rules.

What rule has to be employed, it can not be decided from the theoretical view point. It may be rather determined from the comparison of results with experimental facts. But, overlapping divergences appear in general only in the higher order approximations and so to make such comparisons is hardly expected at the present stage of theory and experiment. When a specific rule is adopted by which we have to carry through the whole calculations, the finite remainder may be uniqely determined as has been shown by Salam in his recent paper[4].

Now, by taking a simple example of overlapping divergence we shall compare the treatments of Salam and Ward. Suppose that a graph, having external variables p, contains in its interior an overlap of two logarithmically divergent parts with respect to variables t_1 and t_2 and diverges as a whole, too (Fig. 1). Corresponding to this graph, we have the following matrix element

Fig. 1.

$$M(p)=\int dt_1 \int dt_2 F(p,t_1)\,G(p,t_1,t_2)\,H(p,t_2). \quad (7)$$

From this expression (7) Salam's method separates and then drops at first the divergences corresponding to t_1 and t_2 sub-integrations:

$$\left.\begin{aligned} &\int dt_2 D(t_1)\,H(p,t_2) && \text{for } t_1 \text{ sub-integration,}\\ \text{and}\quad &\int dt_1 F(p,t_1)\,D(t_2) && \text{for } t_2 \text{ sub-integration,}\end{aligned}\right\} \quad (8)$$

where D's are diverging constant given by $D(t_1)=\int dt_1 F(p_0,t_1)\,G(p_0,t_1,t_{20})$ and $D(t_2)=\int dt_2 G(p_0,t_{10},t_2)\,H(p_0,t_2)$ and t_{10} and t_{20} free momenta corresponding to t_1 and t_2.

On the other hand, we shall apply the Ward's method, in which overlaps are dissolved by differentiating the matrix element with respect to the mass. With this method, the matrix element is transformed as follows:

$$\begin{aligned} M(p)&=\int_\infty^m dm' \int dt_1 \int dt_2 \frac{\partial}{\partial m'}(FGH)\\ &=\int_\infty^m dm' \int dt_1 \int dt_2 \left\{\frac{\partial F}{\partial m'}GH+F\frac{\partial G}{\partial m'}H+FG\frac{\partial H}{\partial m'}\right\}, \end{aligned} \quad (9)$$

where the first and the third terms involves the divergence of t_2 and t_1 sub-integrations, respectively. Contrary to the Salam's case, the dropped terms corresponding to these sub-integrations t_1 and t_2 are

$$\int_\infty^m dm' \int dt_2 D(t_1)\,\frac{\partial H}{\partial m'} \quad \text{and} \quad \int_\infty^m dm' \int dt_1 \frac{\partial F}{\partial m'}D(t_2), \quad \text{respectively.} \quad (10)$$

Thus, as is evident from (8) and (10), the integral of the final integration in each case differs from the other case by the following expression,

$$J(p)=\int_\infty^m dm' \left\{\int dt_1 F(p,t_1)\,\frac{\partial D(t_2)}{\partial m'}+\int dt_2\,\frac{\partial D(t_1)}{\partial m'}H(p,t_2)\right\}. \quad (11)^{*)}$$

As usual $J(p)$, being a function of external momenta p, is expanded in the form

$$J(p)=J(p_0)+(p-p_0)_\mu \frac{\partial J}{\partial p_\mu}(p_0)+\cdots, \quad (12)$$

---

* In most examples in the renormalizable theory D has k_0 dimension and it appears that $\partial D/\partial m$ is equal to zero. But, in the theories in which it is necessary to introduce cut-off factors in order to remove the divergences this term introduces some ambiguities. An example of such circumstances is found in the problem of self-stress of the electron. When D has other dimension, where Ward's method must be somewhat generalized, similar circumstances occur.

where we see that $J(p)$ contributes not only to the divergent part to be removed away, but also to the finite remainder. Here, the following fact is to be noted: in general F and H are reduced integrals and have the same number of external lines as the original graph, and so in the expansion (12) divergences appear to the term of the same order in p as other parts of the final integration. From this example, we may say in general that these two methods do not necessarily lead to the identical results.

Further we shall add a remark on the rule of the separation of divergences. To extract divergent parts from a diverging expression it is usual to make the Taylor expansion with respect to $(p-p_0)_\mu$ in the way as in (12), where p's are external momenta and p_0's the corresponding free ones satisfying $p_0^2+\varkappa^2=0$, say. To make such a separation of divergences is of sufficient physical ground when the separated divergences have simple physical meanings such as the mass or the charge, while in general cases there is not so strong theoretical basis in employing such an expansion. We may separate the divergences by use of other expansion, e.g., the Maclaurin expansion with respect to p's. It is then evident that according as we use the different expansions we shall obtain the results with the different finite contributions (which may be however often compensated by suitably adjusting the coupling constants of counter terms).* In this connection, the best example is found in the graphs as shown in Fig. 2, that is, the graph with two external lines of spin zero fields ϕ^i and ϕ^j, say, which belong to different kinds of field, respectively. $(i \neq j)$. The corresponding matrix element M contains quadratic and logarithmic divergences. In such a case, it is not legitimate to expand M in power of $(\Box-\varkappa^2)$, for in general $\varkappa_i \neq \varkappa_j$. Furthermore, contrary to the usual treatment it is no longer possible to renormalize the latter divergence into the propagation functions of ϕ^i or ϕ^j. As will be shown in the following section it is convenient to renormalize this divergence into the two vertex $V_{ij}=f_{ij}\partial_\mu\phi^i\partial_\mu\phi^j$.** Thus, corresponding to this treatment we have to expand M in power of $\Box$. This is the symmetrical treatment for both fields. In general there occur the similar cases in which it is required to expand the diverging expression in such a way that each separated term is of the same form as the corresponding counter term. Further example will be found in § 4 in connection with the 4-vertex part of c_a-charged field and A^a-field, where the special attention is also required. Thus, according to circumstances we have in general to employ the suitable rules of the separation of divergences.

Fig. 2.

As evident from the above discussions, the finite results are usually dependent on the details of the renormalization rules, and so when carrying through the calculation we must at first prescribe the rules in an unambiguous way. The general considerations developed in the following sections are, however, equally valid whatever rules may be employed.

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* Note added in proof: Similar problems have also been considered by A. Thellung, Helv Phys. Acta **25** (1952), 307.

** In treating such a graph, corresponding to the use of different counter terms, there are many possible renormalization methods, e.g., we may expand M in the form $A+B_i(\Box-\varkappa_i^2)+B_j(\Box-\varkappa_j^2)+\cdots$ and use the corresponding counter terms.

§ 3. Renormalization

Divergences appearing in the S-matrix, when isolated by some appropriate method, are of the same operator forms as one of those which have already been beforehand introduced in the interaction Hamiltonian (6). Therefore, if we take the coupling constants of (6) as $f=f_1+\delta f$, $\lambda=\lambda_1+\delta\lambda$, etc.,* these divergences are cancelled out by the infinite parts δf, $\delta\lambda$, etc., and so the results can be written in terms of the finite coupling constants f_1, λ_1, etc., to give the finite remainder. This method, to be termed the "self consistent subtraction", was discussed in our previous paper[1]. On the other hand, we know another method, in which, as was done by Dyson[3], only the finite remainders are taken into account by simply dropping off the divergences, whose contributions are shown to be equivalent to "renormalizing" the coupling constants f, λ, etc., into f_1, λ_1, etc. In the following paragraph we shall show the outline of the latter method and there it will become evident that aforementioned two prescription of renormalization give the identical results if in treating the divergent terms the same rule is adopted for both cases.

As was shown in the reference 1, the order of divergence of a diverging term $G(E, N, M)$ is given by

$$K_k-\sum_l n_l K_l\,, \tag{13}$$

where notations are the same as in the reference 1 and $K_l \geq 0$ for all the interactions (6). From (13) we see that a primitive divergent graph has at most four external lines. In the graphs with two external lines $\sum E=2$, of ϕ- or ψ-fields two kinds of divergent terms are contained such as $\phi^i\phi^j$ and $\partial_\mu\phi^i\partial_\mu\phi^j$ or $\bar{\psi}^\alpha\psi^\beta$ and $\bar{\psi}^\alpha\gamma_\mu\partial_\mu\psi^\beta$, corresponding to generalizations of mass term when $i\neqq j$ or $\alpha\neqq\beta$ and describing the transformations of elementary particles. In the case of neutral vector fields A^a, however, the divergences are restricted to the form $F^a_{\mu\nu}F^b_{\mu\nu}$ from the arguments of gauge invariancy. On the other hand, the graphs G with $\sum E\leq 3$ contain only one kind of divergent terms. These facts are evident from the Lorentz covariancy.

In our general discussion it is convenient to employ the Ward's method[5] in treating the overlapping divergences. Of course, when we use other method various divergent constants and finite remainders will take different values from the present ones, while it is expected that the proof will be made along a similar line.

For our present purpose it is sufficient as usual to start with the consideration of the connected graphs. Now, let us consider a diverging graph with external lines $\sum E\leq 4$ and let the corresponding matrix element be G. In general, G can be obtained from the corresponding irreducible graphs by inserting various corrections. Here, we use the notation $\langle G\rangle$ to imply that the finite functions to some order of approximation have been inserted in the irreducible graphs. When G contains in its construction some overlapping divergences, we separate them by the Ward's method** and then make the above-mentioned

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* In this paper the renormalized charge is specified by the suffix 1.

** In the general cases of renormalizable theory, Ward's method must be slightly generalized. See Appendix III.

insertions of finite parts. In such a case we use $\langle \bar{G} \rangle$ in place of $\langle G \rangle$.

Next, we shall consider a graph with two external lines. First, we take up the case of ϕ- and ψ-fields. When two external lines refer to the same field, two divergent terms in this graph are respectively renormalizable as usual into the mass and the propagation function. On the contrary, when two free operators refer to different fields, the divergence of the higher order can be cancelled as before by the counter terms $\phi^i\phi^j (i \neq j)$ or $\bar{\psi}^\alpha\psi^\beta (\alpha \neq \beta)$ describing the transformation process, while the lower order one can no longer be renormalizable into the propagation functions. Thus, in our cases the latter divergences are either cancelled by two-vertices $V_{ij}=\lambda_{ij}\partial_\mu\phi^i\partial_\mu\phi^j$ and $V_{\alpha\beta}=\lambda_{\alpha\beta}\bar{\psi}^\alpha\gamma_\mu\partial_\mu\psi^\beta$ or renormalized into the coupling constants of two-vertices λ_{ij} and $\lambda_{\alpha\beta}$. Since in the general renormalizable theories two-vertex parts introduce new peculiar features, we set up the renormalization prescription as follows: The propagation function of ϕ^i-field is modified only by the contributions of the proper self energy parts (two-vertex) part V'_{ii} such as shown in Fig. 3, while the contributions from the graphs such as Fig. 4, though having both end lines referring to the same field ϕ^i, are to be omitted here. Under our rules, the latter contributions are considered as the

Fig. 3

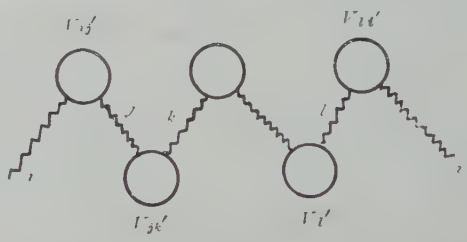

Fig. 4

effect of inserting various two-vertex parts V'_{ij}, $V'_{jk}, \cdots V'_{li}$ in the internal line of ϕ^i. Therefore, when we construct in general a higher order graph with field corrections from the irreducible graph, we have not only to replace the internal lines by corresponding modified propagation functions, but also to make corrections to these lines by inserting two-vertex parts $V'_{ij} (i \neq j)$ to the desired order in various possible combinations. In the same way we can treat the case of ψ^α-fields.

In the case of A^a-fields, the counter term $g_{ab}F^a_{\mu\nu}F^b_{\mu\nu}$ can be treated in the same way as above. In order to see, in the case of $a=b$, its equivalence with the renormalization of coupling constants, we have only to modify this term into the following form:

$$\frac{1}{2}g_{ab}F^a_{\mu\nu}F^b_{\mu\nu}=g_{ab}\{-\varkappa_a^2A^a_\nu A^a_\nu+(\partial_\mu A^a_\nu\partial_\mu A^a_\nu+\varkappa_a^2A^a_\nu A^a_\nu)-\partial_\mu A^a_\nu\partial_\nu A^a_\mu\}.$$

In this expression, the first and the second terms can be renormalized as usual into the mass and the propagation functions of A^a-field, respectively, while the last term does not contribute to the virtual A^a-lines on account of conservation of current. That is, as far as the virtual lines are concerned, only the diagonal terms with respect to vector suffices μ give contributions. Therefore, the discussions of the propagation function can be performed in just the same way as the ϕ^ifields. In the case of two external A^a-lines the last term is rewritten, by the subsidiary condition (3), in the form $-g_{ab}\varkappa_a^2B^{a2}$. This term is to be renormalized into the mass of B^a-fields.

In other respects, the usual procedures are immediately applied with slight modifications.

As usual, the modified propagation functions of field i, α and α and the finite functions of various vertex-parts can be constructed. We have the integral equations:

$$\left.\begin{aligned} &\Delta_F'^{i \text{ or } \alpha'} = \Delta_F^{i \text{ or } \alpha} + \Delta_F^{i \text{ or } \alpha} \sum^{i \text{ or } \alpha *} \Delta_F'^{i \text{ or } \alpha'}, \\ &S_F'^{\alpha'} = S_F^{\alpha} + S_F^{\alpha} \sum^{\alpha *} S_F'^{\alpha'}, \\ &V_{ij\cdots\alpha}' = V_{ij\cdots\alpha} + W_{ij\cdots\alpha}, \end{aligned}\right\} \tag{14}$$

where $\Delta_F^{i \text{ or } \alpha}$, S_F^{α}; $\Delta_F'^{i \text{ or } \alpha'}$ and $S_F'^{\alpha'}$ imply the propagation functions and the corresponding modified ones for fields ϕ^i (or A^α) and ψ^α, respectively, $\sum^{i \text{ or } \alpha *}$ and $\sum^{\alpha *}$ the proper self energy parts of them and $V_{ij\cdots\alpha}$ and $W_{ij\cdots\alpha}$ the vertex factor and the corresponding proper vertex part with external lines of fields $i, j, \cdots$ and α. Considering the order of divergences and taking account of their Lorentz transformation properties we can obtain the finite parts of $\sum^*$'s and V''s as follows:

$$\left.\begin{aligned} &\sum_c^{i \text{ or } \alpha *}(p) = \langle \overline{\sum}^{i \text{ or } \alpha *}(p) \rangle - \frac{1}{8}(p^2 + \varkappa_{i \text{ or } \alpha}^2) \left\langle \frac{\partial^2 \overline{\sum}^{i \text{ or } \alpha *}(p)}{\partial p_\mu \partial p_\mu} \right\rangle (p'), \\ &\sum_c^{\alpha *}(p) = \langle \overline{\sum}^{\alpha *}(p) \rangle - \frac{1}{4}(p\gamma - i\varkappa_\alpha)\gamma_\mu \left\langle \frac{\partial \overline{\sum}^{\alpha *}(p)}{\partial p_\mu} \right\rangle (p'), \\ &V_{ij\cdots\alpha,c}(p_1, p_2, \cdots) = V_{ij\cdots\alpha} + \langle \overline{W}_{ij\cdots\alpha} \rangle (p_1, p_2, \cdots) - \langle \overline{W}_{ij\cdots\alpha} \rangle (p_1', p_2', \cdots) \\ &\qquad - \left\langle \left(\frac{\partial}{\partial p_1} + \frac{\partial}{\partial p_2} + \cdots \right) \overline{W} \right\rangle (p_1', p^{2\prime} \cdots), \end{aligned}\right\} \tag{15}$$

where p''s are in most cases free momenta*). In $\sum^*$'s, the highest divergences (quadratic or logarithmic) have already been cancelled by the mass counter terms and in the case of two-vertices the similar cancellations are achieved by the counter terms of transformation processes. Thus, we find that in each case of the above expression it is sufficient to subtract formally only one diverging term on the right hand side. Hence, V_c's turn out to be of the form

$$V_{ij\cdots\alpha,c} = V_{ij\cdots\alpha} + \langle \overline{W}_{ij\cdots\alpha}(p) \rangle - W_{ij\cdots\alpha} V_{ij\cdots\alpha}, \tag{16}$$

where $W_{ij\cdots\alpha}$'s are logarithmically diverging constants. As the divergent terms of V's are proportional to the corresponding vertex factors V's, these can be removed or absorbed by their coupling constants f's of the corresponding vertices. (Subtraction or renormalization method.)

Finite parts of the modified propagation functions satisfy the following integral equations:

$$\left.\begin{aligned} &\Delta_{Fc}^{i \text{ or } \alpha} = \Delta_F^{i \text{ or } \alpha} + \Delta_F^{i \text{ or } \alpha} \sum_c^{i \text{ or } \alpha *} \Delta_{Fc}^{i \text{ or } \alpha}, \\ &S_{Fc}^{\alpha} = S_F^{\alpha} + S_F^{\alpha} \sum_c^{\alpha *} S_{Fc}^{\alpha}. \end{aligned}\right\} \tag{17}$$

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* See the remark given at the end of § 2.

Now, we shall put as follows:

$$\left.\begin{aligned} &V_{ij\cdots\alpha}{}' = Z_{ij\cdots\alpha}^{-1} V_{ij\cdots\alpha,c}(f_1,\cdots), \\ &\Delta_F^{i \text{ or } \alpha\prime} = Z_{2 \text{ or } 3}^{i \text{ or } \alpha} \Delta_{Fc}^{i \text{ or } \alpha}(f_1,\cdots), \\ &S_F^{\alpha\prime} = Z_2^{\alpha} S_{Fc}^{\alpha}(f_1,\cdots), \\ &f_{ij\cdots\alpha,1} = (Z_2^i Z_2^j \cdots Z_2^{\alpha})^{1/2} Z_{ij\cdots\alpha}^{-1} f_{ij\cdots\alpha}, \text{ etc.} \end{aligned}\right\} \tag{18}$$

If it is possible to determine the constants Z's by inserting the ansatz (18) in integral equations, we are then led to the desired result that the subtraction procedure is reinterpreted or justified in terms of the renormalization of constants.

In making such insertions, there holds the following rule for the calculation of Z factors: As an example, we shall consider a vertex part $W_{ij\cdots\alpha} = M_{ij\cdots\alpha}(f)/f_{ij\cdots\alpha}$, where M is the corresponding matrix element. When we insert the ansatz in this expression, M is transformed as follows,

$M_{ij\cdots\alpha}(f) = \langle \bar{M}_{ij\cdots\alpha}(f_1) \rangle / (Z_2^i Z_2^j \cdots Z_2^{\alpha})^{1/2} = Z_{ij\cdots\alpha}^{-1} f_{ij\cdots\alpha} \langle \bar{M}_{ij\cdots\alpha}(f_1) \rangle / f_{ij\cdots\alpha,1}$. And so, we see that $W_{ij\cdots\alpha}(f) = Z_{ij\cdots\alpha}^{-1} \langle \bar{M}_{ij\cdots\alpha}(f_1) \rangle / f_{ij\cdots\alpha,1} = Z_{ij\cdots\alpha}^{-1} \langle \bar{W}_{ij\cdots\alpha,1}(f_1) \rangle$. Similarly, we also have the relation $\sum^{i*}(f) = (Z_2^i)^{-1} \langle \bar{\sum}^{i*}(f_1) \rangle$.

Inserting (18) in (14), considering the above rules and then comparing these equations with (16) and (17), we get

$$\left.\begin{aligned} &Z_{2 \text{ or } 3}^{i \text{ or } \alpha} = 1 + \frac{1}{2\pi i} \frac{1}{8} \left\langle \frac{\partial^2 \bar{\sum}^{i \text{ or } \alpha}(p)}{\partial p_\mu \partial p_\mu} \right\rangle (p'), \\ &Z_2^{\alpha} = 1 + \frac{1}{2\pi} \frac{1}{4} \gamma_\mu \left\langle \frac{\partial \bar{\sum}^{\alpha *}(p)}{\partial p_\mu} \right\rangle (p'), \\ &Z_{ij\cdots\alpha} = 1 + W_{ij\cdots\alpha}. \end{aligned}\right\} \tag{19}$$

Thus, we have established our desired result that the subtraction procedure is in general equivalent to the renormalization of coupling constants.

§ 4. On the observable electric charge

Among the renormalized coupling constants the most interesting ones are those of the electric charges e_0 or, in general, e_α's. The empirical fact of charge conservation is expressed in the gauge invariancy of the theory. In order that the non-singular theory is not in conflict with this empirical fact, it is required that the renormalized theory is also invariant for the transformation (5) with $e_{0,1}^i$, $e_{0,1}^{\alpha}$ replacing e_0^i, e_0^{α}, respectively, or in speaking in terms of the subtraction method, that the counter terms, each of which has been separately determined so as to compensate the individual divergence, are gauge invariant as a whole. The corresponding requirement must also be satisfied for the charges e_α's in general. In this section, we shall show that by the renormalization prescriptions stated in the foregoing section we can obtain, in fact, a theory satisfying such requirements. It

is expected, however, that for the reason given in § 2 the renormalized charge may take different values according as we adopt different renormalization rules.

We shall denote, in general, the 3-vertex and 4-vertex factors representing the interaction of $e_a (a=0, 1, \cdots)$ charged particle i (or a) with one and two A^a-lines by $V_\mu^{i,a}(p_1, p_2)$ and $V_{\mu\nu}^{i,ab}(p_1, p_2, l)$ and the corresponding vertex parts by $W_\mu^{i,a}$ and $W_{\mu\nu}^{i,ab}$, respectively, where p_1, p_2 and l are momenta of charged and A lines incident on the vertices. In terms of the propagation function $S_F(p)$*, the free field equation of the e_a-charged particle is given by

$$S_F^{-1}(p)\psi(p)=0. \tag{20}$$

Taking into account the facts that the gauge invariant vector interactions with A_μ^a are to be introduced in (20) by replacing p_μ by $(p-\sum e_a A^a)_\mu$ and that coefficients of $e_a A_\mu^a$ and $e_a e_b A_\mu^a A_\nu^b$ give V_μ^a and $V_{\mu\nu}^{ab}$, respectively, we get the following useful relations

$$\left.\begin{aligned} V_\mu^{i,a}(p, p) &= -S_F^{-1}(p)\frac{\partial S_F(p)}{\partial p_\mu}S_F^{-1}(p), \\ V_{\mu\nu}^{i,ab}(p, p, 0) &= \frac{1}{2}\frac{\partial V_\mu^{i,a}(p, p)}{\partial p_\nu}. \end{aligned}\right\} \tag{21}$$

These relations express the relations between the propagation function and the vertex factors at which zero momentum A-lines ($l=0$) are incident.

Differentiating the proper self energy part of e_a-charged particle i (or ') as shown in Fig. 5 with respect to external momentum p_μ and considering (21), we obtain in general

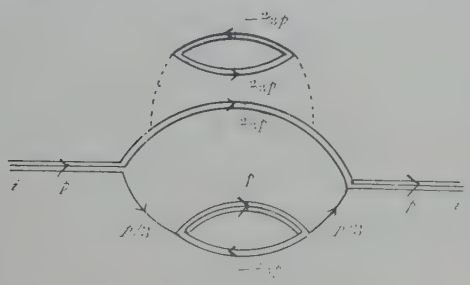

Fig. 5

represents lines with charges 0, e_a, $2e_a$, $3e_a$, respectively.

$$-\frac{1}{2\pi i}\frac{\partial \sum^{i*}(p)}{\partial p_\mu}=\Pi_\mu^{i,a}(p, p). \tag{22}$$**

Because, in the integrand of $\sum^*$, we can appropriately choose the momentum variables so that the external momentum p always follows the main charged lines, which never vanishes halfway for the reason of e_a-charge conservation, and so the differentiation with respect to p_μ changes a part of these lines into a 3-vertex with zero momentum A_μ^a line incident. Here, it should be noticed that by attaching the external momentum p to the charged lines in such a way as shown in Fig. 5, i.e., distributing p to each charged line in proportion to the magnitude of its charge, we can get 3-vertices with the weighting factors proportional to the magnitudes of the respective e_a-charges. In general,

* As to the general discussion of the propagation function, see the forthcoming paper by Y. Takahashi and one of the present authors (H.U.), in press.

** The factor i is necessary for Bose fields.

further contributions to the 3-vertex parts come from those graphs in which the zero momentum A^a-line is incident on the e_a-charged loops created by virtual neutral ($e_a=0$) lines. From the requirement of gauge invariancy, however, such a contribution is always proportional to $F^a_{\mu\nu}$ of zero momentum A^a-line and so does not contribute to $\Pi'^a_\mu(p, p)$. Thus, (22) holds in general. Further, rewriting $\sum^*$ as $\sum^*(p+q)$ and attaching the momentum q to the e_b-charged lines in proportion to the magnitudes of e_b-charges as above we get similarly

$$W^{i,ab}_{\mu\nu}(p, p, 0) = \frac{1}{2}\frac{\partial W^{i,a}_\mu(p, p)}{\partial p_\nu}. \tag{23}$$

As is evident from the above derivations, (22) and (23) are always valid whatever interactions there may be.

Now, we shall apply these results to the specific cases of the renormalizable fields. Of course, there is no 4-vertices for spinor fields. For the particles with e_a and e_b charges the vertex parts Π'^a_μ and $\Pi'^{ab}_{\mu\nu}$ etc. diverge logarithmically, while for the particles without e_a and e_b charges the corresponding graphs converge from the general arguments of the gauge invariance with respect to A^a- and A^b-fields*). The relations (18) are in this case written in the following forms;

$$\left.\begin{aligned} &V^{i,a'}_\mu = (Z_1^{i,a})^{-1} \Gamma^{i,a}_{\mu,c}(f_1), \quad \Gamma'^{i,a'}_{\mu\nu} = (Z_1^{i,a})^{-1} V^{i,a}_{\mu\nu,c}(f_1), \\ &\Gamma'^{i,ab'}_{\mu\nu} = (Z_4^{i,ab})^{-1} V^{i,ab}_{\mu\nu,c}(f_1); \\ &V^{\alpha,a'}_\mu = (Z_1^{\alpha,a})^{-1} V^{\alpha,a}_{\mu,c}(f_1), \quad \Delta'^{a'}_F = Z_3^a \Delta^a_{F,c}(f_1), \end{aligned}\right\} \tag{24}$$

and

$$\left.\begin{aligned} &e^i_{a,1} = (Z_3^a)^{1/2}(Z_1^{i,a})^{-1} Z_2^i e^i_a, \quad [(e^i_a)^2]_1 = Z_3^a (Z_4^{ia})^{-1} Z_2^i (e^i_a)^2, \\ &(e^i_a e^i_a)_1 = (Z_3^a Z_3^b)^{1/2}(Z_4^{i,ab})^{-1} Z_2^i (e^i_a e^i_b); \\ &e^\alpha_{a,1} = (Z_3^a)^{1/2}(Z_1^{\alpha,a})^{-1} Z_2^\alpha e^\alpha_a. \end{aligned}\right\} \tag{25}$$

To extract the diverging parts from Π'_μ's and $\Pi'_{\mu\nu}$'s, we expand them in powers of p_1 and p_2.**) Then we find the infinite constants Π''s as defined by (16) as follows;

$$\left.\begin{aligned} &W^{i,a}_\mu = \frac{1}{8}\left\langle \frac{\partial \bar{W}^{i,a}_\lambda(p, p)}{\partial p_\lambda} \right\rangle (p'), \\ &W^{i,a}_{\mu\nu} = W^{i,ab}_{\mu\nu} = \frac{1}{4}\langle \bar{W}^{i,a}_{\lambda\lambda}(p, p_2, 0) \rangle (p'), \\ &W^{\alpha a}_\mu = \frac{1}{4}\gamma_\lambda \langle \bar{W}^{\alpha,a}_\lambda(p, p) \rangle (p'). \end{aligned}\right\} \tag{26}$$

* When the use is made of the renormalization method of coupling constants, we take $\lambda_{ii}=\lambda_{\alpha\alpha}=0$ in (6) as usual.

** It should be noticed that we have to subtract from $\Gamma'_{\mu\nu}$ the diverging constant $\bar{\Pi}'_{\lambda\lambda}(p', p', 0)$ instead of $\bar{W}_{\lambda\lambda}(p', p', l'')$ with $l''^2=\varkappa^2$, for when expanding in $(l-l'')$ the contributions to the charge of $A_\mu{}^a A_\mu{}^b$ vertex come from terms of higher power in e'.

Considering the fact that two operations $\partial/\partial m^i$ and $\partial/\partial p$ are commutable and so there holds the relations $\langle \partial \sum^{i*}(p)/\partial p_\mu \rangle = \langle \partial \sum^{i*}(p)/\partial p_\mu \rangle$, etc. and taking into accout the relations (22), (23), (26) and (19), we find

$$\left.\begin{aligned} &Z_1^{i,a} = Z_2^i = Z_4^{i,a} = Z_4^{i,ab}, \\ &Z_1^{\alpha,a} = Z_2^\alpha, \end{aligned}\right\} \tag{27}$$

which correspond to the generalization of the Ward's identity[6].

Inserting the above relations in (25) we finally obtain

$$\left.\begin{aligned} &e_{a1}^i = (Z_3^a)^{1/2} e_a^i, \quad [(e_a^i)^2]_1 = (e_{a,1}^i)^2, \\ &[e_a^i e_b^i]_1 = e_{a,1}^i e_{b,1}^i, \quad e_{a,1}^\alpha = (Z_3^a)^{1/2} e_a^\alpha. \end{aligned}\right\} \tag{28}$$

This result shows that there are units for renormalized charges, too. If in particular for the electric charges we put $e_0^i = e_0^\alpha = e$ for the mechanical charge, we get

$$e_{0,1}^i = e_{0,1}^\alpha = (Z_3^0)^{1/2} e, \tag{28'}$$

that is, the renormalized electric charges of all the elementary particles take the same value $e_{0,1}$. From these results, we may say as follows: The self-charges of charged particles are due only to the photon proper-fields equally interacting with all the charged particles in the nature. Thus, all the charged particles have the same self-charges[7][8].

In order to obtain these relations, it is necessary, as is evident from their derivations, that we have to use consistently the same rule of renormalization so as to preserve the relationships between self energy parts and vertex parts such as (22) and (23) throughout the calculations.

Next, we shall consider the graphs having two free operators of different fields $i \neq j$ (or $\alpha \neq \beta$) and zero, one or two A^a lines incident thereupon. Corresponding to these divergences, we have introduced in (6) the following interactions or counter terms;

$$\left.\begin{aligned} &\lambda_{ij} \partial_\mu \phi^{i*} \partial_\mu \phi^j, \; i\lambda_{ij} A_\mu^a \{e_a^i \phi^{i*} \partial_\mu \phi^j - e_a^j \partial_\mu \phi^{i*} \phi^j\}, \\ &\lambda_{ij} e_a^i e_b^j \phi^{i*} \phi^j A_\mu^a A_\mu^b, \\ &\lambda_{\alpha\beta} \bar{\psi}^\alpha \gamma_\mu \partial_\mu \psi^\beta, \; -i\lambda_{\alpha\beta} A_\mu^a e_a^\beta \bar{\psi}^\alpha \gamma_\mu \psi^\beta, \text{ etc.} \end{aligned}\right\} \tag{29}$$

As already mentioned in the previous section, after the higher order divergences are cancelled by $f_{ij}\phi^{i*}\phi^j$, $f_{\alpha\beta}\bar{\psi}^\alpha\psi^\beta$, etc., the remaining divergences will be renormalized into λ_{ij}, $\lambda_{ij}^a = \lambda_{ij} e_a^i$, $\lambda_{ij}^{ab} = \lambda_{ij} e_a^i e_b^j$ and $\lambda_{\alpha\beta}$, $\lambda_{\alpha\beta}^a = \lambda_{\alpha\beta} e_a^\beta$, respectively. Let the contributions from respective graphs be $\sum^{ij*}$, $\Pi_\mu^{ij,a}$ and $V_{\mu\nu}^{ij,ab}$ etc., respectively. Then from the similar relations as (22) and (23) and the ansatz

$$\left.\begin{aligned} &V^{ij\prime} = (Z_5^{ij})^{-1} V_e^{ij}, \; V_\mu^{ij,a\prime} = (Z_1^{ij,a})^{-1} V_{\mu,e}^{ij,a}, \\ &V_{\mu\nu}^{ij,ab\prime} = (Z_4^{i,a})^{-1} V_{\mu\nu,e}^{ij,a}, \; V_{\mu\nu}^{ij,ab\prime} = (Z_4^{ij,ab})^{-1} V_{\mu\nu,e}^{ij,ab}; \\ &V^{\alpha\beta\prime} = (Z_5^{\alpha\beta})^{-1} V_e^{\alpha\beta}, \; V_\mu^{\alpha\beta,a\prime} = (Z_1^{\alpha\beta,a})^{-1} V_{\mu,e}^{\alpha\beta,a}, \end{aligned}\right\} \tag{30}$$

and

$$\left.\begin{aligned}
&\lambda_{ij,1}=(Z_1^{ij})^{-1}(Z_2^{i}Z_2^{j})^{1/2}\lambda_{ij},\quad \lambda^{a}_{ij,1}=(Z_2^{ij,a})^{-1}(Z_2^{i}Z_2^{j})^{1/2}(Z_3^{a})^{1/2}\lambda^{a}_{ij},\\
&\lambda^{ab}_{ji,1}=(Z_4^{ij,ab})^{-1}(Z_2^{i}Z_2^{j})^{1/2}(Z_3^{a}Z_3^{b})^{1/2}\lambda^{ab}_{ij}\ ;\\
&\lambda_{\alpha\beta,1}=(Z_5^{\alpha\beta})^{-1}(Z_2^{\alpha}Z_2^{\beta})^{1/2}\lambda_{\alpha\beta},\quad \lambda^{a}_{\alpha\beta,1}=(Z_1^{\alpha\beta,a})^{-1}(Z_2^{\alpha}Z_2^{\beta})^{1/2}(Z_3^{\alpha})^{1/2}\lambda^{a}_{\alpha\beta},
\end{aligned}\right\}\quad (31)$$

we get again

$$\left.\begin{aligned}
&Z_5^{ij}=Z_1^{ija}=Z_4^{ij,ab},\\
&Z_5^{\alpha\beta}=Z_1^{\alpha\beta a},
\end{aligned}\right\}\quad (32)$$

and so we find

$$\left.\begin{aligned}
&\lambda_{ij,1}=(Z_5^{ij})^{-1}(Z_2^{i}Z_2^{j})^{1/2}\lambda_{ij},\quad \lambda^{a}_{ij,1}=\lambda_{ij,1}e^{i}_{a,1},\\
&\lambda^{ab}_{ij,1}=\lambda_{ij,1}e^{i}_{a,1}e^{j}_{b,1}\ ;\\
&\lambda_{\alpha\beta,1}=(Z_5^{\alpha\beta})^{-1}(Z_2^{\alpha}Z_2^{\beta})^{1/2}\lambda_{\alpha\beta},\quad \lambda^{a}_{\alpha\beta,1}=\lambda_{\alpha\beta,1}e^{\beta}_{a,1}.
\end{aligned}\right\}\quad (33)$$

That is, the interrelations between the coupling constants of the interaction in (29) are simply rewritten in terms of renormalized constants after the renormalization. Therefore, from (28) and (33) we find that the renormalized non-singular theory is invariant under the gauge transformation (5) with replacements $e_a^{i \text{ or } \alpha} \to e_{a,1}^{i \text{ or } \alpha}$, or in other words a set of gauge invariant counter terms is able to cancel the individual divergent terms. It should be remembered, however, that this invariancy of the whole theory is guaranteed for the first time when the renormalization is carried through by noticing the aforementioned points.

§ 5. Concluding remarks

So far our considerations have been referred to the consistency of the renormalizable field theory by postponing to touch the deeper questions relating to the fundamentals of the theory itself, that is, the convergency of the perturbation series and the divergent nature of the renormalization constants. In order that the theory is completely rational, it is required that the perturbation series converges and furthermore that divergences do not appear in the renormalization constants. In this section we shall briefly examine these problems.

First, we shall consider the perturbation series in the quantum electrodynamics. Let $N_M(n)$ be the number of independent Feynman graphs in the n-th order approximation, describing a certain transition M. In general, it is easily found that $f_M(n)=N_M(n+2)/N_M(n)$ increases with increasing n. Thus, when the weight factor is left out of consideration, the ratio of the contributions of $(n+2)$-th order to those of n-th order becomes larger than 1 for the values on n as given by $f_M(n)>137$. Therefore, unless the more graphs compensate each other for the larger value of n, the perturbation series will not converge and so it will no longer be possible to interpret the splendid successes in the lower order calculations in the quantum electrodynamics*). In this connection it should be noted further that if there were the interaction of the 2nd kind in the nature such an interpretation

* Note added in proof: The detailed discussion concerning this problem has recently been given by C. A. Hurst, Proc. Roy. Soc. 214 A (1952) 44.

not be admissible either, because then the quantum electrodynamics would not be renormalizable.

Even if the perturbation series converges, there still remains the divergences in the renormalization constants. Notwithstanding its mathematical incompleteness, the renormalization procedure, dealing with the diverging quantities is guaranteed or given a theoretically rational basis only when these divergences are shown to be not essential ones, but merely of the apparent nature.

Concerning to the finiteness of the renormalized charge, Thirring[9] has recently presented an interesting consideration. Previously[8], we have also suggested a similar possibility, that is, the requirement that the self-charge should be finite as a whole would give a condition for the numerical value of $e_{0,1}^2/\hbar c$, which should be a root with even multiplicity of some equation $f(e_{0,1}^2/\hbar c)=0$.

On the other hand, however, it seems also probable that the very reason or the deep meaning of what the success of the renormalization theory in the quantum electrodynamics implies may not be found within the renormalization theory itself, but rather in the profound and more essential foundations which support and underlie the present field theories.

The authors wish to express their cordial thanks to Prof. S. Sakata for his continued interest and valuable discussions.

Appendix 1

On the Interactions between the charged field Q_α and the electromagnetic field A_μ or the neutral vector field U_μ with mass $\varkappa$.

We shall use in this and the following sections the bold letters and the usual letters for the quatities in the Heisenberg- and interaction-representations respectively. If $\boldsymbol{J}_\mu$ is the electric current in the Heisenberg representation ;

$$\boldsymbol{J}_\mu=-\frac{\partial \boldsymbol{L}}{\partial \boldsymbol{A}_\mu} \tag{I·1}$$

$$=-ie\left(\frac{\partial \boldsymbol{L}}{\partial \boldsymbol{Q}_{\alpha;\mu}}\boldsymbol{Q}_\alpha-\boldsymbol{Q}_\alpha^*\frac{\partial \boldsymbol{L}}{\partial \boldsymbol{Q}_{\alpha;\mu}^*}\right), \tag{I·1}'$$

we can derive the important relation

$$J_\mu(x)\equiv[S(\sigma)\boldsymbol{J}_\mu(x)S^{-1}(\sigma)]_{x/\sigma}=\frac{\partial H(x\,;n)}{\partial A_\mu}. \tag{I·2}$$

In order to prove this relation, we shall introduce the independent canonical variables of the charged field :

$$Q_\alpha(x)=S(\sigma)\boldsymbol{Q}_\alpha(x)S^{-1}(\sigma), \tag{I·3}$$

$$P_\alpha(x)=\frac{\partial L}{\partial Q_{\alpha;\mu}}n_\mu=S(\sigma)\frac{\partial \boldsymbol{L}}{\partial \boldsymbol{Q}_{\alpha;\mu}}S^{-1}(\sigma)n_\mu, \tag{I·4}$$

and put

$$Q_{\alpha;\mu}(x)=S(\sigma)\boldsymbol{Q}_{\alpha;\mu}S^{-1}(\sigma)+C_{\alpha;\rho}n_\mu n_\rho\,. \tag{I·5}$$

Then we have from (I·4)

$$H(x,\,n)=S(\sigma)\boldsymbol{T}_{\mu\nu}S^{-1}(\sigma)n_\mu n_\nu-T_{\mu\nu}n_\mu n_\nu \tag{I·6}$$

$$=S(\sigma)\left\{\frac{\partial \boldsymbol{L}}{\partial \boldsymbol{Q}_{\alpha;\mu}}\boldsymbol{Q}_{\alpha;\nu}+\boldsymbol{Q}^*_{\alpha;\nu}\frac{\partial \boldsymbol{L}}{\partial \boldsymbol{Q}^*_{\alpha;\mu}}-\delta_{\mu\nu}\boldsymbol{L}\right\}S^{-1}(\sigma)n_\mu n_\nu$$

$$-\frac{\partial L}{\partial Q_{\alpha;\mu}}Q_{\alpha;\nu}n_\mu n_\nu-Q^*_{\alpha;\nu}\frac{\partial L}{\partial Q^*_{\alpha;\mu}}n_\mu n_\nu-L^0$$

$$=C_{\alpha;\nu}\frac{\partial L}{\partial Q_{\alpha;\mu}}n_\mu n_\nu+C^*_{\alpha;\nu}\frac{\partial L}{\partial Q^*_{\alpha;\mu}}n_\mu n_\nu+S(\sigma)\boldsymbol{L}S^{-1}(\sigma)-L^0. \tag{I·6}'$$

On the other hand, we have from (I·1)

$$J_\mu=\frac{\partial}{\partial A_\mu}(S(\sigma)\boldsymbol{L}S^{-1}(\sigma))+S(\sigma)\frac{\partial \boldsymbol{L}}{\partial \boldsymbol{Q}_{\alpha;\rho}}S^{-1}(\sigma)n_\rho n_\nu\frac{\partial C_{\alpha;\nu}}{\partial A_\mu}$$

$$+S(\sigma)\frac{\partial \boldsymbol{L}}{\partial \boldsymbol{Q}^*_{\alpha;\rho}}S^{-1}(\sigma)n_\rho n_\nu\frac{\partial C^*_{\alpha;\nu}}{\partial A_\mu}. \tag{I·7}$$

Comparing (I·6)′ and (I·7) and taking into account (I·4), we get the relation (I·2).

Let

$$J_\mu\equiv j_\mu+j_{\mu\nu}A_\nu, \tag{I·8}*$$

then we obtain from (I·2)

$$H(x\,;\,n)=j_\mu A_\mu+\frac{1}{2}j_{\mu\nu}A_\mu A_\nu+H'(x), \tag{I·9}$$

where $H'(x)$ is the part which does not contain A_μ-field. (I·9) is the important relation between the current and the electric interaction.

Using (I·1)′ and (I·4), we can easily prove the relation

$$J_4=j_4,\ \text{i.e.,}\ j_{\mu\nu}n_\nu=0. \tag{I·10}$$

On the other hand, the Lagrangian of the vector interaction between the charged fields U_μ can be obtained from the Lagrangian of the electromagnetic interaction by replacing A_μ with U_μ.

Moreover we have

$$\boldsymbol{U}_\mu(x)=S(\sigma)\left\{U_\mu(x)+\frac{1}{\varkappa^2}J_\nu(x)n_\mu n_\nu\right\}S^{-1}(\sigma), \tag{I·11}$$

because

$$_4=\frac{i}{\varkappa^2}\partial_k P_k\,,\qquad P_k\equiv U_{k4}=\frac{\partial L}{\partial U_{k;\mu}}n_\mu,$$

---

* j_μ and $j_{\mu\nu}$ do not contain A_ρ.

$$\boldsymbol{U}_4=\frac{i}{\varkappa^2}\partial_k \boldsymbol{P}_k-\frac{1}{n^2}\boldsymbol{J}_4, \quad \boldsymbol{P}_k\equiv\boldsymbol{U}_{k4}=\frac{\partial \boldsymbol{L}}{\partial \boldsymbol{U}_{k;\mu}}n_\mu, \quad (k=1,2,3)$$

where $\boldsymbol{U}_k$ and $\boldsymbol{P}_k$ are independent canonical variables and so

$$\boldsymbol{U}_k=S(\sigma)U_kS^{-1}(\sigma), \quad \boldsymbol{P}_k=S(\sigma)P_kS^{-1}(\sigma).$$

From (I·11), (I·9), and (I·10) one obtains

$$H(x;n)=j_\mu U_\mu+\frac{1}{2}j_{\mu\nu}U_\mu U_\nu+\frac{1}{2\varkappa^2}(j_\mu n_\mu)^2+H'(x). \tag{I·12}^{*)}$$

The current $\boldsymbol{J}_\mu$ satisfies the continuity-equation :

$$\partial_\mu \boldsymbol{J}_\mu=0. \tag{I·13}$$

In the interaction representation, the continuity equation (I·13) will be transformed into the following form :

$$\partial_\mu J_\mu(x)=i\int[j_\mu(x), H(x';n)]\,d\sigma_\mu'. \tag{I·14}$$

Comparing the terms with the same power of U_μ in the both sides of (I·14), we obtain the following relations :**)

$$\partial_\mu j_\mu(x)=i\int[j_\mu(x), H'(x')]\,d\sigma_\mu', \tag{I·15}$$

$$\left.\begin{aligned} &n_\mu[j_\mu(x), j_\nu(x')]=in_\mu\partial_\rho\partial_\mu\Delta(x'-x)\,j_{\rho\nu}(x'),\\ &n_\mu n_\nu[j_\mu(x), j_\nu(x')]=0,\\ &n_\mu[j_\mu(x), j_{\rho\nu}(x')]=0. \end{aligned}\right\} \tag{I·16}$$

In the Stueckelberg's formalism for the neutral vector field we have the relations :

$$\left.\begin{aligned} &U_\mu=A_\mu+\frac{1}{\varkappa}\partial_\mu B,\\ &(\partial_\mu A_\mu+\varkappa B)\,\Psi[\sigma]=0. \end{aligned}\right\} \tag{I·17}$$

Introducing the unitary transformation

$$\left.\begin{aligned} &\Psi[\sigma]\to\Psi'[\sigma]=T^{-1}[\sigma]\Psi[\sigma],\\ &T[\sigma]\equiv\exp\left[-\frac{i}{\varkappa}\int_\sigma j_\mu(x')B(x')d\sigma_\mu'\right], \end{aligned}\right\} \tag{I·18}$$

and using (I·15) and (I·16), we obtain the following Schrödinger equation and supplementary condition :

---

* In (I·12), we also take into account the fact that the free Lagrangian of the U_μ-field gives $(-1/2\varkappa^2)\times(j_\mu n_\mu)^2$ in the course of unitary transformation (I·6).

** The some examples of (I·15) are given in Appendix II.

$$\left[i\frac{\delta}{\delta\sigma(x)}-j_\mu A_\mu-\frac{1}{2}j_{\mu\nu}A_\mu A_\nu-H'(x)\right]\Psi'[\sigma]=0,$$
$$[\partial_\mu A_\mu+\varkappa B-\int_\sigma j_\mu(x')\Delta(x-x')d\sigma_\mu']\Psi'[\sigma]=0. \tag{I·19}$$

(I·19) gives in the limit $\varkappa\to 0$ the Schrödinger equation and the Lorentz condition in the quantum electrodynamics for the arbitrary charged fields (generalized Glauber's theorem[2]). The above theorem can be easily extended to the case in which many charged fields and neutral vector fields are present simultaneously.

Appendix II

Firstly we treat the case of the gauge-invariant interaction between the many spinor fields $\psi^\alpha(\alpha=1, 2,\cdots)$ and the electromagnetic field A_μ:

$$L'=\lambda_{\alpha\beta}\bar{\psi}^\alpha\gamma_\mu\partial_\mu\psi^\beta-ie(\delta_{\alpha\beta}+\lambda_{\alpha\beta})A_\mu\bar{\psi}^\alpha\gamma_\mu\psi^\beta. \tag{II·1}$$

Accroding to the method of reference 10 we have from (II·1):

$$\psi^\alpha(x)=S(\sigma)\psi^\alpha(x)S^{-1}(\sigma),\quad A_\mu(x)=S(\sigma)A_\mu(x)S(\sigma)^{-1},$$
$$\bar{\psi}^\alpha(x)=S(\sigma)\bar{\psi}^\alpha(x)S^{-1}(\sigma) \tag{II·2}$$
$$+\frac{1}{2}\int[\{\lambda_{\alpha\beta}\bar{\psi}^{\alpha'}\gamma_\mu\partial_\mu+ie(\delta_{\alpha\beta}+\lambda_{\alpha\beta})A_\mu'\bar{\psi}^{\alpha'}\gamma_\mu\}(\gamma\partial-\varkappa),\ \varepsilon(x-x')]\Delta(x-x')dx'$$
$$=S(\sigma)\bar{\psi}^\alpha S(\sigma)^{-1}+\lambda_{\beta\alpha}\bar{\psi}^\beta\gamma_\mu\gamma_\nu n_\mu n_\nu, \tag{II·3}$$

where dash refers to the point x' and x is on σ.

We have from (II·3):

$$(\delta_{\beta\alpha}+\lambda_{\beta\alpha})\bar{\psi}^\beta=S(\sigma)\bar{\psi}^\alpha S^{-1}(\sigma). \tag{II·4}$$

The interaction Hamiltonian $H(x\,;n)$ can be obtained from the following relations:

$$S(\sigma)[\bar{\psi}^\alpha(x), H(x'\,;n)]S^{-1}(\sigma)$$
$$=i\{\lambda_{\alpha\beta}\bar{\psi}^{\alpha'}\gamma_\mu\partial_\mu+ie(\delta_{\alpha\beta}+\lambda_{\alpha\beta})A_\mu'\bar{\psi}^{\alpha'}\gamma_\mu\}(\gamma\partial-\varkappa)\Delta(x-x'),$$
$$S(\sigma)[\psi^\alpha(x), H(x'\,;n)]S^{-1}(\sigma)$$
$$=i(\gamma\partial-\varkappa)\Delta(x-x')\{\lambda_{\alpha\beta}\gamma_\mu\partial_\mu\psi^\beta-ie(\delta_{\alpha\beta}+\lambda_{\alpha\beta})A_\mu\gamma_\mu\psi^\beta\}, \tag{II·5}$$
$$S(\sigma)[A_\mu(x), H(x'\,;n)]S^{-1}(\sigma)$$
$$=-i\Delta(x-x')\bar{\psi}^\alpha\gamma_\mu\psi^\alpha$$

for x/σ and x'/σ.

Substituting (II·2) and (II·3) into (II·5) we have the following interaction Hamiltonian:

$$H(x\,;n)=-ie\,\psi^\alpha\gamma_\mu A_\mu\psi^\alpha+\varkappa\lambda_{\alpha\beta}\,g_{\beta\gamma}\bar{\psi}^\alpha\psi^\gamma, \tag{II·6}$$

where

$$g_{\alpha\beta}(\lambda_{\beta\gamma}+\delta_{\beta\gamma})=\delta_{\alpha\gamma}. \tag{II·7}$$

It should be noted that the interaction $\bar{\psi}^{\alpha}\gamma_{\mu}A_{\mu}\psi^{\beta}$ $(\alpha\neq\beta)$ connecting different charged fields does not appear in (II·6). This simple circumstance, however, does not hold for the cases of charged spinless fields.

In spite of the above result (II·6) we can use (II·1) as the interaction Hamiltonian when we replace the P-brackets by the Green functions and neglect the normal dependent terms appearing in the course of the calculation.

For the interaction Lagrangian between the many scalar fields ϕ^{i} and the electromagnetic field A_{μ}:

$$\begin{aligned}\boldsymbol{L}'=&\lambda_{ij}\partial_{\mu}\boldsymbol{\phi}^{i*}\partial_{\mu}\boldsymbol{\phi}^{j}+i(\delta_{ij}+\lambda_{ij})e\boldsymbol{A}_{\mu}(\boldsymbol{\phi}^{i*}\partial_{\mu}\boldsymbol{\phi}^{j}-\partial_{\mu}\boldsymbol{\phi}^{i*}\boldsymbol{\phi}^{j})\\&-(\delta_{ij}+\lambda_{ij})e^{2}\boldsymbol{A}_{\mu}\boldsymbol{A}_{\mu}\boldsymbol{\phi}^{i*}\boldsymbol{\phi}^{j},\end{aligned} \tag{II·8}$$

we can obtain the following interaction Hamiltonian, along the same line as the spinor case:

$$\begin{aligned}H(x\,;n)=&-\lambda_{ij}(\partial_{\mu}\phi^{i*}\partial_{\mu}\phi^{j}+\partial_{\mu}\phi^{i*}\partial_{\nu}\phi^{j}n_{\mu}n_{\nu})\\&-(g_{ij}-\delta_{ij})\partial_{\mu}\phi^{i*}\partial_{\nu}\phi^{j}n_{\mu}n_{\nu}\\&+(\delta_{ij}+\lambda_{ij})ieA_{\mu}(\partial_{\mu}\phi^{i*}\phi^{j}-\phi^{i*}\partial_{\mu}\phi^{j})\\&+ie\lambda_{ij}A_{\mu}(\partial_{\nu}\phi^{i*}\phi^{j}-\phi^{i*}\partial_{\nu}\phi^{j})n_{\mu}n_{\nu}\\&+e^{2}(\delta_{ij}+\lambda_{ij})(A_{\mu}A_{\mu}+A_{\mu}A_{\nu}n_{\mu}n_{\nu})\phi^{i*}\phi^{j}\end{aligned} \tag{II·9}$$

where g_{ij} is defined by

$$g_{ij}(\lambda_{jk}+\delta_{jk})=\delta_{ik}. \tag{II·10}$$

Comparing (II·9) with (I·12), we have $H'(x)$ containing no coupling constant e:

$$\begin{aligned}H'(x)=&-\lambda_{ij}(\partial_{\mu}\phi^{i*}\partial_{\mu}\phi^{j}+\partial_{\mu}\phi^{i*}\partial_{\nu}\phi^{j}n_{\mu}n_{\nu})\\&-\partial_{\mu}\phi^{i*}(g_{ij}-\delta_{ij})\partial_{\nu}\phi^{j}n_{\mu}n_{\nu}.\end{aligned} \tag{II·11}$$

On the other hand, the current J_{μ} is:

$$\begin{aligned}&J_{\mu}=j_{\mu}+j_{\mu\nu}A_{\nu},\\&j_{\mu}=ie(\delta_{ij}+\lambda_{ij})(\partial_{\mu}\phi^{i*}\phi^{j}-\phi^{i*}\partial_{\mu}\phi^{j})\\&\qquad+ie\lambda_{ij}(\partial_{\nu}\phi^{j*}\cdot\phi^{j}-\phi^{i*}\partial_{\nu}\phi^{j})n_{\mu}n_{\nu}\\&j_{\mu\nu}=2e^{2}(\delta_{ij}+\lambda_{ij})(\delta_{\mu\nu}+n_{\mu}n_{\nu})\phi^{i*}\phi^{j}\end{aligned} \tag{II·12}$$

It is easily seen from (II·12) that this $j_{\mu\nu}$ satisfies (I·10). Using (II·11) and (II·12) we can easily establish the continuity equation (I·15). These relations give the examples of the general discussions in Appendix I.

Appendix III

In this section we shall be concerned with the generalization of Ward's method.[5] In our case the generalization becomes necessary in the following two points : i) there appear linear divergences which can not be made convergent by performing the operation $\partial/\partial m$ (below); and ii) some of the coupling constants have the dimensions of mass or $(\text{mass})^2$, which may introduce the factor m (below) into the Z-factors.

In order to remove these difficulties we modify the method as follows : We put, as done by Ward, $\varkappa_i = m\mu_i$ and further, for the coupling constants having dimensions, $f_i = mg_i$, $f_j = m^2 g_j$, $\cdots$, where μ_i, g_i, g_j, $\cdots$ are of no dimensions. For a graph containing some overlapping divergences, we can dissolve these by several times differentiating with respect to m, $(\partial/\partial m)^l$ (l is determined for the given graph). If the first of differentiations removes an overlap, this term is to be treated in just the same way as Ward. When the first differentiation operates on the linearly diverging part or on the coupling constants f_i, f_j, $\cdots$, in order to dissolve the overlaps we have to make the second differentiation for this term. Proceeding in this way successively, we can dissolve all the overlapping parts. For the terms in which the overlaps have already been treated, the remaining differentiations $(\partial/\partial m)^{l'}$ $(l' < l)$ become trivial. As we have put $f_i = mg_i$, $f_j = mg_j$, $\cdots$, the difficulty (ii) disappears automatically. In other respects we can proceed in the same way as Ward.

References

1) S. Sakata, H. Umezawa and S. Kamefuchi, Phys. Rev. **84** (1951), 154; Prog. Theor. Phys. **7** (1952), 377.
2) H. Umezawa, Prog. Theor. Phys. **7** (1952), 551.
3) F. J. Dyson, Phys. Rev. **75** (1949), 1736.
4) A. Salam, ibid. **82** (1951), 217, **84** (1951), 426.
5) J. C. Ward, Proc. Roy. Soc. **A64** (1951), 54; Phys. Rev. **84** (1951), 897.
6) J. C. Ward, Phys. Rev. **78** (1950), 182.
7) H. Umezawa and E. Yamada, Prog. Theor. Phys. **4** (1949), 251.
8) H. Umezawa and S. Kamefuchi, ibid. **6** (1951), 543.
9) W. E. Thirring, Zeit. f. Naturforsch. **6a** (1951), 462.
10) Y. Takahashi and H. Umezawa, Prog. Theor. Phys. in press.

Errata

Y. Takahashi and H. Umezawa **On the Self-stress**

(Prog. Theor. Phys. **8** (1952), 193)

The right hand sides of Eqs. (4·9) and (4·10) should be multiplied by 2.

The right hand sides of Eqs. (4·11) and (4·12) should be devided by 2.

The right hand sides of Eqs. (A·4), (A·5) and (A·6) should be multiplied by $\varkappa^2$, μ and μ, respectively.

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On the Equivalence of the Particle Formalism and the Wave Formalism of Meson

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We have shown that Dyson-Feynman's S matrix for the meson-photon dynamical system in the β-formalism is equivalent to that in the wave formalism, explicitly. For this purpose, we use the Fujiwara's formulation concerning with the β-matrix. We drop off the bilinear terms in the electromagnetic field with use of the modified propagation function of meson and so the Feynman diagrams in the β-formalism consist only of the 3-vertices. On the contrary, the diagrams in the wave formalism consist of 4-vertices as well as 3-vertices. In spite of this apparent difference of both formalisms, the equivalence is complete.

§ 1. Introduction

Recently, many authors[1),2),3)] have discussed the interaction of meson with the electromagnetic field using the β-formalism. This formalism is attractive on account of the following two reasons: *the one is its analogy with the spinor field and the other its synthesis of the scalar- and vector-meson theories.* But these advantages are destroyed when we treat the interaction of meson with nucleon, for the interaction can not be introduced in an elegant way.[4)] However, this defect was much improved recently by several authors,[5),6),7),8)] and the wave aspects can be discussed by the β-formalism, too. Though all kind of problems concerning with meson can be treated in the β-formalism, there are no cases at present that this formalism is especially advantageous. But for the tentative research of the Bose field in which its particle aspects is accented, the β-formalism might be a better mathematical technique. So we shall clarify the connection between the β-formalism and the Klein-Gordon's or Proca's formalism.

Seeing Duffin's derivation of his equation,[9)] we can infer that the equations of motion in both formalisms are equivalent. But it is rather dependent upon the special representation of β-matrix. Recently, this equivalence is discussed by Harish-Chandra,[5)] Fujiwara[10)] and others[7),11)] independent by of the representation of the β-matrix. In this paper, we show explicitly the equivalence of the S matrices in both formalisms drawn down by the Feynman-Dyson's graphical method.

In both formalisms, the interaction of meson with the electromagnetic field contains the linear and bilinear terms in the electromagnetic field. However, *in the case of the*

β formalism, the bilinear terms (the surface dependent and independent) can be removed by the P'-technique of Kinoshita,[2] *and the modified propagation function of meson is used*[2),3),12]. *Thus the Feynman diagrams consist only of the 3-vertices and the analogy to the spinor electrodynamics is complete.* On the contrary, in the case of the wave formalism, the corresponding P^*-technique can only remove the surface dependent bilinear term but not the surface independent one. Then the Feynman diagrams consist of 4-vertices as well as 3-vertices, and the number of diagrams corresponding to any process becomes greater than the former case. In this point, the β-formalism is superior to the wave formalism. *In spite of this remarkable difference, the S matrix in the β-formalism using the modified propagation function of meson coincids perfectly with the one in the wave formalism, as shown below.*

For the purpose of our discussion, it is convenient to use the Fujiwara's formulation, and so we summarize his results in § 2. In § 3 and § 4, we treat the interaction of scalar or vector meson with the electromagnetic field, respectively. After the first draft of this paper was completed, we received A. Salam's paper[15] published on the Proc. Roy. Soc., in which the similar formulas as ours appear in an incomplete form.

§ 2. Some results of Fujiwara's formulation

At first, we summarize the Fujiwara's results concerned with the β-formalism of meson. In this formalism, free meson is expressed by the matrix of 16-rows and 1-column $\psi(x)$ and satisfies the following Duffin-Kemmer equation of motion

$$(\beta\partial+\varkappa)\psi(x)=0, \tag{1}$$

where $\varkappa$ is the mass of the meson, and $\beta\partial\equiv\sum_{\mu=1}^{4}\beta_\mu\frac{\partial}{\partial x_\mu}$ $\left(\partial_\mu=\frac{\partial}{\partial x_\mu},\ x_4=it\right)$. Natural unit system $\hbar=c=1$ is used throughout this paper. Hereafter, we shall omit the summation symbol $\sum$ for dummy suffices as usual so long as the contrary is not expressed. Also these suffices themselves are omitted when no confusion arises. β_μ's are hermitian matrices satisfying the following algebraic relation

$$\beta_\mu\beta_\nu\beta_\lambda+\beta_\lambda\beta_\nu\beta_\mu=\delta_{\mu\nu}\beta_\lambda+\delta_{\lambda\nu}\beta_\mu\,. \tag{2}$$

Define the adjoint $\bar{\psi}(x)$ of $\psi(x)$ by

$$\bar{\psi}(x)=\psi^*(x)\eta_4\,, \tag{3}$$

where $\psi^*(x)$ is a complex conjugate of $\psi(x)$ and

$$\eta_\mu=2\beta_\mu{}^2-E \qquad \text{(no summation)}. \tag{4}$$

E is a unit matrix.

$\bar{\psi}(x)$ satisfies the following equation of motion,

$$\partial\bar{\psi}(x)\beta-\varkappa\bar{\psi}(x)=0. \tag{5}$$

As is well known,[16] β_μ is a reducible 16-rowed square matrix and have just two

non-trivial irreducible sub-matrices, the 5-rowed square sub-matrix corresponding to the scalar meson and the 10-rowed corresponding to the vector meson. Henceforward, we consider two cases separately, but *β-matrices themselves which appear in each case are not the sub-matrices but the original 16-rowed ones.*

(i) *Scalar Case*

Define

$$P=\beta_\mu{}^2\beta_\nu{}^2\beta_\lambda{}^2\beta_\sigma{}^2 \qquad \text{(no summation)}, \tag{6}$$

where μ, ν, λ and σ are 1, 2, 3 or 4 but differ to each other. P does not depend upon the order of the suffices μ's for $\beta_\mu{}^2$'s commute with each other. P is such a matrix that $P\psi(x)$ transforms as a scalar for a Lorentz-transformation, so P may be called a scalar projector in this meaning. Thus, put

$$P\psi(x)=\sqrt{x}\,U(x)=\begin{pmatrix} \vdots \\ \cdots\cdots \\ \sqrt{x}\,u(x) \\ \vdots \end{pmatrix}. \tag{7}$$

(Dot denotes zero.)

Notice that $U(x)$ is not a simple function but a matrix. The last matrix represents the concrete form of $U(x)$ when we use the Kemmer's representations of β_μ's. Though our discussion is independent of the special representation, this representation assists our understanding of $P\psi(x)$. $u(x)$ corresponds to the scalar wave function of the wave formalism and satisfies the Klein-Gordon equation of motion. Similarly,

$$P_\mu=\beta_\mu P\beta_\mu \qquad \text{(no summation)} \tag{8}$$

is a vector projector, signifying that $P_\mu\psi(x)$ transforms as a vector for a Lorentz transformation. Define

$$\bar{P}=\sum_\mu P_\mu=\beta_\mu P\beta_\mu\,, \tag{9}$$

then

$$E^s=\bar{P}+P=\beta_\mu P\beta_\mu+P=\begin{pmatrix} 0 & \vdots & 0 & 0 \\ \cdots & \vdots & \cdots & \cdots \\ 0 & \vdots & 1_1\,0\,1_1 & 0 \\ & \vdots & 0\;\;1_1 & \\ \cdots & \vdots & \cdots & \cdots \\ 0 & \vdots & 0 & 0 \end{pmatrix}, \tag{10}$$

i.e., E^s is a unit matrix for the 5-rowed sub-matrix, but other elements are all zero. Then E^s projects the original β_μ's on the 5-rowed sub-space. The properties of P and $\bar{P}$ are as follows:

$$P^2=P, \qquad \bar{P}^2=\bar{P}, \tag{11}$$

$$P\beta_\mu\beta_\nu=\beta_\mu\beta_\nu P=\delta_{\mu\nu}P, \tag{12}$$

$$P\beta_\mu=\beta_\mu\bar{P}, \qquad \bar{P}\beta_\mu=\beta_\mu P, \tag{13}$$

$$P=\frac{1}{4}\beta_\mu\bar{P}\beta_\mu, \tag{14}$$

$$P\underbrace{\beta_\mu\cdots\cdots\beta_\nu}_{\text{odd number}}P=\bar{P}\underbrace{\beta_\mu\cdots\cdots\beta_\nu}_{\text{odd number}}\bar{P}=0, \tag{15}$$

$$SpP=SpP_\mu=1, \qquad Sp\bar{P}=4. \tag{16}$$

Now we compare our notations with other authors. P and $\bar{P}$ relate with the notations of Harish-Chandra,[7] Salam[16] and Peaslee[5] as follows:

Fujiwara	Harish-Chandra	Salam	Peaslee
P	$\frac{1}{4}\beta_\mu\beta\beta_\mu$	X	$\frac{M-1}{3}$
$\bar{P}$	β	Y	$\frac{4-M}{3}$

(17)

where $M=\beta_\mu\beta_\mu$. But they (except Harish-Chandra) did not consider an individual P_μ. Moreover, ours refer to an original 16-rowed matrix but others to a 5-rowed sub-matrix.

(ii) *Vector Case*

Define

$$R_\mu=(1-\beta_\mu^2)\beta_\nu^2\beta_\lambda^2\beta_\sigma^2 \qquad \text{(no summation)}, \tag{18}$$

where μ's are same as scalar case. R_μ is such a matrix that transforms as a vector for a Lorentz transformation, i.e., R_μ is a vector projector. Put

$$R_\mu\psi(x)=\sqrt{\varkappa}\,U_\mu(x)=\begin{pmatrix}\vdots\\ \sqrt{\varkappa}\,u_\mu(x)\leftarrow\mu\text{-th}\\ \vdots\end{pmatrix} \tag{19}$$

where $U_\mu(x)$ is also not a simple function but a matrix. The last term represents the concrete form of $U_\mu(x)$ when we use the Kemmer's representations of β_μ's. $u_\mu(x)$ corresponds to the vector wave function of the wave formalism. Similarly,

$$R_{(\mu\nu)}=\beta_\mu R_\nu\beta_\mu=\beta_\nu R_\mu\beta_\nu \qquad \text{(no summation)} \tag{20}$$

is a tensor projector, signifying that $R_{(\mu\nu)}\psi(x)$ transforms as a tensor for a Lorentz transformation. $(\mu\nu)$ shows that $R_{(\mu\nu)}$ is symmetric in μ and ν. Define

$$R=\sum_{\mu} R_{\mu}\,, \tag{21}$$

$$\bar{R}=\sum_{\mu>\nu} R_{(\mu\nu)}=\frac{1}{2}\sum_{\mu,\nu}\beta_{\mu}R_{\nu}\beta_{\mu}\,, \tag{22}$$

for the last reformation, next relations

$$R_{\mu}\beta_{\mu}=\beta_{\mu}R_{\mu}=0 \qquad \text{(no summation)} \tag{23}$$

(obtained from (18)) are used. Then

$$E^{v}=\bar{R}+R=\frac{1}{2}\sum_{\mu,\nu}\beta_{\mu}R_{\nu}\beta_{\mu}+\sum_{\mu}R_{\mu} \tag{24}$$

is a unit matrix only of the 10-rowed submatrix and projects the original β_{μ}'s on the 10-rowed sub-space. The properties of R and $\bar{R}$ are as follows;

$$R^2=R, \qquad \bar{R}^2=\bar{R}, \tag{25}$$

$$R\beta_{\mu}=\beta_{\mu}\bar{R}, \qquad \bar{R}\beta_{\mu}=\beta_{\mu}R, \tag{26}$$

$$R_{\mu}=\beta_{\nu}R_{(\mu\nu)}\beta_{\nu}\,, \qquad \text{(no summation)} \tag{27}$$

$$R\underbrace{\beta_{\mu}\cdots\cdots\beta_{\nu}}_{\text{odd number}}R=\bar{R}\underbrace{\beta_{\mu}\cdots\cdots\beta_{\nu}}_{\text{odd number}}\bar{R}=0, \tag{28}$$

$$\bar{R}\underbrace{\beta_{\mu}\cdots\cdots\beta_{\lambda}}_{\text{even number}}R=R\underbrace{\beta_{\mu}\cdots\cdots\beta_{\lambda}}_{\text{even number}}\bar{R}=0. \tag{29}$$

For the calculation hereafter, it is convenient to define the following matrix

$$Q_{\mu\nu}=\delta_{\mu\nu}E-\beta_{\nu}\beta_{\mu}\,, \tag{30}$$

where E is a unit matrix of a total matrix. Also define

$$R_{\mu\nu}=R_{\mu}Q_{\mu\nu} \qquad \text{(no summation)}, \tag{31}$$

then using (23) we have

$$R_{\mu\mu}=R_{\mu}\,. \qquad \text{(no summation)} \tag{32}$$

R and $\bar{R}$ are represented by $R_{\mu\nu}$ as follows:

$$R=\delta_{\mu\nu}R_{\mu\nu}\,, \tag{33}$$

$$\bar{R}=\frac{1}{2}\delta_{\lambda\rho}\delta_{\mu\nu}\beta_{\lambda}R_{\mu\nu}\beta_{\rho}\,. \tag{34}$$

$R_{\mu\nu}$ have the following properties;

$$R_{\mu\nu}R_{\lambda\rho}=\delta_{\nu\lambda}R_{\mu\rho}\,, \tag{35}$$

$$\left.\begin{aligned}\beta_{\lambda}\beta_{\rho}R_{\mu\nu}&=\delta_{\lambda\rho}R_{\mu\nu}-\delta_{\lambda\mu}R_{\rho\nu}\\ R_{\mu\nu}\beta_{\lambda}\beta_{\rho}&=\delta_{\lambda\rho}R_{\mu\nu}-\delta_{\nu\rho}R_{\mu\lambda}\end{aligned}\right\}, \tag{36}$$

$$R_{\mu\nu}\beta_\tau\beta_\xi R_{\lambda\rho}=(\delta_{\tau\xi}\delta_{\nu\lambda}-\delta_{\tau\lambda}\delta_{\nu\xi})R_{\mu\rho}\,, \tag{37}$$

$$SpR_{\mu\nu}=\delta_{\mu\nu}\,, \tag{38}$$

$$\left.\begin{aligned} R_{\mu\nu}\psi(x)&=\sqrt{\varkappa}\,U_{\mu\nu}(x)=\begin{pmatrix}\vdots\\ \sqrt{\varkappa}\,u_\nu(x)\\ \vdots\end{pmatrix}\leftarrow \mu\text{-th},\\ \bar{\psi}(x)R_{\mu\nu}&=\sqrt{\varkappa}\,U_{\mu\nu}{}^*(x)=(\cdots\cdots\sqrt{\varkappa}\,u_\mu{}^*(x)\cdots\cdots)\,.\\ &\qquad\qquad\qquad\qquad\uparrow\\ &\qquad\qquad\qquad\qquad\nu\text{-th}\end{aligned}\right\} \tag{39}$$

§ 3. The interaction of scalar meson with the electromagnetic field

We show explicitly that the S matrix of Dyson and Feynman for the interaction of meson with the electromagnetic field in the β-formalism is equivalent to that in the wave formalism. In this section, we calculate for the case of scalar meson, and in the following for that of vector meson.

The interaction Hamiltonian for this case (both for scalar and vector mesons) is given by

$$H(x)=-ie\bar{\psi}(x)\beta_\mu\psi(x)A_\mu(x),$$

where $A_\mu(x)$ is the electromagnetic field variable. In the usual covariant formalism, the interaction Hamiltonian contains the terms bilinear in $A_\mu(x)$, (surface dependent and independent), but as shown by several authors[2),3),12)], we can ignore this interaction parts by modifying the propagation function of meson. We follow this treatment in this paper.

$\psi(x)$ satisfies

$$(\beta\partial+\varkappa)\psi(x)=0. \tag{1}$$

Multiplying (1) by $\bar{P}=\beta_\nu P\beta_\nu$ from left side, we get

$$-\varkappa\beta_\nu P\beta_\nu\psi=\beta_\nu P\beta_\nu(\beta\partial)\psi\,.$$

Using (12), this can be rewritten:

$$\beta_\nu P\beta_\nu\psi=-\frac{1}{\varkappa}(\beta\partial)P\psi\,.$$

Adding $P\psi$ in both sides and using (10), we obtain lastly

$$\psi^s(x)=-\frac{1}{\varkappa}(\beta\partial-\varkappa)P\psi(x), \tag{40}$$

where $\psi^s = E^s \psi$ and we have non-vanishing elements only in the scalar (5-rowed) part. Similarly,

$$\bar{\psi}^s(x) = \frac{1}{\varkappa} \bar{\psi}(x) P(\beta \overleftarrow{\partial} + \varkappa), \tag{41}$$

where $\overleftarrow{\partial}$ operates on $\bar{\psi}(x)$, and $\bar{\psi}^s$ is the hermitian conjugate of ψ^s.

Commutation relations for the field variables contained in (33) are (both for scalar and vector mesons)

$$[\psi_\rho(x), \bar{\psi}_\sigma(x')] = \frac{1}{i} \left\{ \beta\partial - \frac{1}{\varkappa} (\beta\partial)^2 \right\}_{\rho\sigma} \Delta(x-x'), \tag{42}$$

$$[A_\mu(x), A_\nu(x')] = i \delta_{\mu\nu} D(x-x'), \tag{43}$$

others are zero.

(42) can be reformed for the scalar meson as follows:

$$[\psi_\rho^s(x), \bar{\psi}_\sigma^s(x')] = \frac{1}{i} (\bar{P}+P) \left\{ \beta\partial - \frac{1}{\varkappa} (\beta\partial)^2 \right\}_{\rho\sigma} (\bar{P}+P) \Delta(x-x')$$

$$= \frac{i}{\varkappa} (\beta\partial - \varkappa) P(\beta\partial - \varkappa)_{\rho\sigma} \Delta(x-x'). \tag{44}$$

In this reformation, relation (9), (12), (15) and

$$(\Box - \varkappa^2) \Delta(x-x') = 0 \tag{45}$$

are used. (44) are also obtained from relation (7) and the commutation relation of the Klein-Gordon wave functions

$$[u(x), u^*(x')] = i\Delta(x-x'). \tag{46}$$

The modified propagation function for meson (both for scalar and vector) is $\frac{1}{2} T_F(x)$ where

$$T_F(x) = -\left\{ \beta\partial - \frac{1}{\varkappa} (\beta\partial)^2 + \frac{1}{\varkappa} (\Box - \varkappa^2) \right\} \Delta_F(x). \tag{47}$$

This can be reformed for the scalar meson in the same way as the commutation relation

$$T_F^s(x) = \frac{1}{\varkappa} \{ (\beta\partial - \varkappa) P(\beta\partial - \varkappa) - \beta_\mu P \beta_\mu (\Box - \varkappa^2) \} \Delta_F(x). \tag{48}$$

The photon propagation function is $\frac{1}{2} \delta_{\mu\nu} D_F(x)$ as usual.

Under these preparations, we consider such graphs G_n which consist of n vertices, E_m external meson lines and E_p external photon lines. The S_n, the n-th order term of S matrix of any process, can be written down according to the following recipe from this graph.

Recipe S_β

1. Draw all connected diagrams with n vertices, E_m external meson lines, and E_p external photon lines.
2. Write down an integral in momentum space for each diagram as follows:

(a) Insert

$$A_\mu(k)$$

for each external photon line,

$$-\frac{1}{\varkappa}(i\beta p-\varkappa)P\psi(p), \tag{49}$$

or

$$-\frac{1}{\varkappa}\bar{\psi}(p)P(i\beta p-\varkappa) \tag{50}$$

for each external meson line pointing into or out of the diagram, respectively.

(b) Insert

$$\delta_{\mu\nu}D_F(k)=\delta_{\mu\nu}\frac{1}{k^2}$$

for each internal photon line,

$$T_F^s(p)=-\frac{1}{\varkappa}\{(i\beta p-\varkappa)P(i\beta p-\varkappa)+\beta_\mu P\beta_\mu(p^2+\varkappa^2)\}/(p^2+\varkappa^2) \tag{51}$$

for each internal (scalar) meson line. (For convenience, the sign is reversed.)

(c) Insert

$$\beta_\mu\delta(p-p'\pm k) \tag{52}$$

for each vertex.

(d) Integrate over all momenta and multiply each integral by the same factor

$$(-i)^n(-i)^{\frac{n-E_p}{2}}i^{-\frac{E_m}{2}}\left(\frac{e}{4\pi^2}\right)^n. \tag{53}$$

3. Sum these integrals.

(49), (50) and (51) are the Fourier transforms of (40), (41) and (48), respectively. In (52), if at one end of an internal photon line the δ-function is (arbitrarily) written with $+k$, the δ-function at the other end of the same internal photon line must be written with $-k$.

Corresponding recipe for Klein-Gordon's scalar meson is given by Rohrlich[14], and in this case some complexities arise by reason of the appearance of 4-vertices as well as 3-vertices. The recipe is as follows:

Recipe S_w

1. Draw all connected diagrams with n 3-vertices, E_m external meson lines, and

E_p external photon lines.

2. Find all possible 4-vertex diagrams by schrinkage of the 3-vertex diagrams.
3. Write down an integral in momentum space for each diagram as follows:

(a) Insert

$$A_\mu(k)$$

for each external photon line,

$$u(p) \quad \text{or} \quad u^*(p) \tag{54}$$

for each external meson line pointing into or out of the diagram respectively.

(b) Insert

$$\delta_{\mu\nu} D_F(k) = \delta_{\mu\nu} \frac{1}{k^2}$$

for each internal photon line,

$$\Delta_F^s(p) = \frac{1}{p^2 + \varkappa^2} \tag{55}$$

for each internal (scalar) meson line.

(c) Insert

$$(p_\mu + p_\mu')\,\delta(p - p' \pm k) \tag{56}$$

for each 3-vertex,

$$-\delta_{\mu\nu}\,\delta(p - p' \pm k \pm k') \tag{57}$$

for each 4-vertex.

(d) Integrate over all momenta and multiply each integral by its respective weight

$$w = 2^g, \qquad g = d - a - b. \tag{58}$$

Multiply each integral by the same factor

$$(-i)^{\frac{n - E_p - E_m}{2}} \left(\frac{e}{4\pi^2}\right)^n. \tag{59}$$

4. Sum these integrals.

In (58), d is the number of 4-vertices, a is the number of closed photon lines (Fig. 1), and b is the number of pairs of 4-vertices connected by two photon lines (Fig. 2).

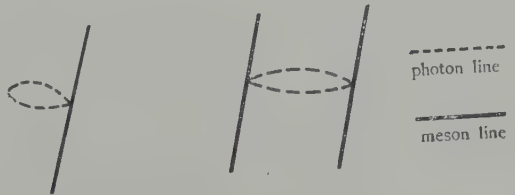

Fig. 1. Fig. 2.

Comparing two recipes, we notice that the same photon factors appear in both ones. Therefore, *to demonstrate the equivalence of the S matrix in both cases it is only necessary to show that the meson factors in S_β reduce to ones in S_w.* This reduction is easily done by treating the typical two or three adjacent meson lines. As $T_F^s(p)$ consists of two parts,

$$\left.\begin{aligned} T_F^{s_1}(p) &= (i\beta p - \varkappa) P \frac{-1/\varkappa}{p^2+\varkappa^2} P(i\beta p - \varkappa), \\ \text{and} \qquad T_F^{s_2}(p) &= -\frac{1}{\varkappa}\beta_\mu P \beta_\mu, \end{aligned}\right\} \tag{60}$$

it appears following three types. Of these

$$\text{(i)} \qquad T_F^{s_2}(p)\beta_\mu T_F^{s_2}(p') = \frac{1}{\varkappa^2}\beta_\lambda P \beta_\lambda \beta_\mu \beta_\nu P \beta_\nu = 0 \tag{61}$$

because of (15). Others are

$$\begin{aligned} \text{(ii)} \quad & T_F^{s_1}(p)\beta_\mu T_F^{s_1}(p') \\ &= (i\beta p - \varkappa) P \frac{-1/\varkappa}{p^2+\varkappa^2} P(i\beta p - \varkappa)\beta_\mu (i\beta p' - \varkappa) P \frac{-1/\varkappa}{p'^2+\varkappa^2} P(i\beta p' - \varkappa) \\ &= (i\beta p - \varkappa) P \frac{-1/\varkappa}{p^2+\varkappa^2} P(-i\varkappa)(p_\mu + p_\mu') \frac{-1/\varkappa}{p'^2+\varkappa^2} P(i\beta p' - \varkappa) \qquad (62) \\ &= (i\beta p - \varkappa) P \frac{-1/\varkappa}{p^2+\varkappa^2} i(p_\mu + p_\mu') \frac{1}{p'^2+\varkappa^2} P(i\beta p' - \varkappa) \end{aligned}$$

and

$$\begin{aligned} \text{(iii)} \quad & \int dq\, T_F^{s_1}(p)\beta_\mu \delta(p - q \pm k)\; T_F^{s_2}(q)\beta_\nu \delta(q - p' \pm k')\; T_F^{s_1}(p') \\ &= (i\beta p - \varkappa) P \frac{-1/\varkappa}{p^2+\varkappa^2} \delta(p - p' \pm k \pm k') P(i\beta p - \varkappa)\beta_\mu \times \\ &\qquad \times \left(-\frac{1}{\varkappa}\right)\beta_\lambda P \beta_\lambda \beta_\nu (i\beta p' - \varkappa) P \frac{-1/\varkappa}{p'^2+\varkappa^2} P(i\beta p' - \varkappa) \\ &= (i\beta p - \varkappa) P \frac{-1/\varkappa}{p^2+\varkappa^2} \delta(p - p \pm k \pm k') P(-\varkappa)\delta_{\mu\lambda}\delta_{\lambda\nu} \frac{-1/\varkappa}{p'^2+\varkappa^2} P(i\beta p' - k) \\ &= (i\beta p - \varkappa) P \frac{-1/\varkappa}{p^2+\varkappa^2} i^2(-\delta_{\mu\nu})\delta(p - p' \pm k \pm k') \frac{1}{p'^2+\varkappa^2} P(i\beta p' - \varkappa). \qquad (63) \end{aligned}$$

In these reductions, relations (11) and (12) are used. For brevity, δ-functions of vertices are omitted in (61) and (62). In (62) and (63), the factors $(p_\mu + p_\mu')\delta(p - p' \pm k)$ and $-\delta_{\mu\nu}\delta(p - p' \pm k \pm k')$ are just equal to the 3-vertex- and 4-vertex-factors (see (56) and (57)), respectively. That is to say, the propagation function has the symmetrical form, for example, $T_F^{s_1}(p)$ consists of three parts $(i\beta p - \varkappa)P$ (L-part), $\dfrac{-1/\varkappa}{p^2+\varkappa^2}$ (M-part)

and $P(i\beta p-\varkappa)$ (R-part) ; and then, the 3-vertex of the wave formalism is given by placing the vertex β_μ between two $T_F^{s_1}$'s and combining β_μ with the R-part of the former $T_F^{s_1}$ and the L-part of the latter, and in the same way the 4-vertex is given by placing the adjacent vertices β_μ and β_ν (put $T_F^{s_2}$ between them) between two $T_F^{s_1}$'s and combining them with the R-part of the former $T_F^{s_1}$ and the L-part of the latter. The M-part gives just the scalar meson propagation function (55) of the wave formalism except the factor $-1/\varkappa$. We can continue this procedure successively for the series of internal meson lines, because of the symmetrical form of the meson propagation function. When the connected meson lines form a closed loop, it remains SpP lastly and

$$SpP=1 \tag{64}$$

from (16). When the connected meson lines form an open polygon, the end meson lines are the external ones and the factors $P(i\beta p-\varkappa)$ or $(i\beta p-\varkappa)P$ of (49) or (50) play the R- or L-part of $T_F^{s_1}$ in the above procedure, and after we have managed the all vertices of the polygon as above, it remains

$$\begin{aligned}\bar{\psi}(p)P\cdots\cdots P\psi(q) &= \sqrt{\varkappa}\,U^*(p)\cdots\cdots\sqrt{\varkappa}\,U(q)\\ &= \varkappa u^*(p)\cdots\cdots u(q),\end{aligned} \tag{65}$$

where relation (7) is used.

Then, for an open polygon, only difference between the S matrices in the β-formalism and that in the wave-formalism is the i-factors and the sign involved in (53) and (59). If we cancel the factor $-\varkappa$ (appearing in the course of calculating (62) and (63)) with the factor $-1/\varkappa$ of M-part of the progagation function placed after the vertex β_μ, then only the leftmost one (coefficient $-1/\varkappa$ of $\bar{\psi}^s(x)$) remain. This factor $1/\varkappa$ just cancels with $\varkappa$ of (64), thus there remains only a factor -1 for each open polygon. For a closed loop, these factors cancel cyclically, and as no external meson lines exist, those complexities as above do not arise. For the process in question, there are just $E_m/2$ open polygons, so they give the factor

$$(-1)^{\frac{E_m}{2}}. \tag{66}$$

Also there appears a factor i to each vertex β_μ in (62) and (63). As there are n vertices, the factor

$$i^n \tag{68}$$

appears. (53) combined with (66) and (67) gives

$$(-i)^{\frac{n-E_p-E_m}{2}}\left(\frac{e}{4\pi^2}\right)^n.$$

This is exactly same as (59). The weight factor (58) is easily obtained by considering that (63) is independent of the exchange of μ and ν (weight 2 to each 4-vertex), but for the cases of Fig. 1 and 2 the Kronecker's δ of the photon propagation function reduces the weight to 1. Thus the equivalence of S matrices for scalar electrodynamics in β-formalism and wave formalism is complete.

From the above consideration, the order of divergence of S matrices is clearly equal for both formalism, and also the number and kind of primitive divergent graphs are equal. This point is recently indicated by Salam[1F)] comparing the highest power of momentum p in the numerator with one in the denominator, employing the formula similar to ours.

§ 4. The interaction of vector meson with the electromagnetic field

In this section, we extend the method of the previous section for the interaction of vector meson with the electromagnetic field. This can be done by slight alterations of the previous consideration.

The vector meson wave function ψ^v and $\bar{\psi}^v$ are written as follows;

$$\psi^v = -\frac{1}{\varkappa}(\beta\partial - \varkappa) R\psi\,, \tag{68}$$

$$\bar{\psi}^v = \frac{1}{\varkappa}\bar{\psi} R(\beta\overleftarrow{\partial} + \varkappa), \tag{69}$$

derived in the same way as the scalar case (put R (or $\bar{R}$) in place of P (or $\bar{P}$)). The commutation relation and propagation function are slightly complicated; i.e.,

$$[\psi^v_\rho(x), \bar{\psi}^v_\rho(x')] = \frac{i}{\varkappa}[(\beta\partial - \varkappa) R(\beta\partial - \varkappa) + \{(\beta\partial)^2 - \varkappa^2\} R]_{\rho\sigma} \Delta(x - x'), \tag{70}$$

$$T^v_F(x) = \frac{1}{\varkappa}[(\beta\partial - \varkappa) R(\beta\partial - \varkappa) - \frac{1}{2}\beta_\mu R \beta_\mu(\Box - \varkappa^2) + \{(\beta\partial)^2 - \Box\} R]\, \Delta_F(x - x'), \tag{71}$$

The differences between scalar and vector case are the appearance of the last term and the factor $1/2$ of the second term. The recipes to write down the S_n are the same as scalar case with some change, that is:

Recipe V_β

Insert

$$-\frac{1}{\varkappa}(i\beta p - \varkappa) R\psi(p), \tag{72}$$

and

$$-\frac{1}{\varkappa}\bar{\psi}(p) R(i\beta p - \varkappa) \tag{73}$$

in place of (49) and (50).

Insert

$$T^v_F(p) = T^{v_1}_F(p) + T^{v_2}_F(p) + T^{v_3}_F(p)$$

$$= -\frac{1}{\varkappa}\Big\{(i\beta p - \varkappa) R(i\beta p - \varkappa) +$$

$$\frac{1}{2}\beta_\mu R\beta_\mu(p^2+\varkappa^2)+p_\rho R_{\rho\sigma}p_\sigma\Big\}\Big/(p^2+\varkappa^2) \tag{74}$$

in place of (51).

The last term of (74) is derived from the Fourier transform of $\{(\beta\partial)^2-\Box\}R$, employing (36)

$$\begin{aligned}-\{(\beta p)^2-p^2\}R&=-\delta_{\mu\nu}\{(\beta p)^2-p^2\}R_{\mu\nu}\\&=-\delta_{\mu\nu}(p^2R_{\mu\nu}-p_\mu p_\rho R_{\rho\nu}-p^2R_{\mu\nu})\\&=p_\rho p_\nu R_{\rho\nu}.\end{aligned}$$

Others are unchanged.

The recipe S_w are altered as follows ;[17]

Recipe V_w

Insert

$$u_\mu(p) \qquad \text{or} \qquad u_\mu^*(p) \tag{75}$$

in place of (54),

$$J_F^\nu(p)=\frac{\delta_{\rho\sigma}+1/\varkappa^2\cdot p_\rho p_\sigma}{p^2+\varkappa^2} \tag{76}$$

in place of (55).

Insert

$$\{\delta_{\rho\sigma}(p_\mu+p_\mu')-\delta_{\mu\rho}p_\sigma+\delta_{\mu\sigma}p_\rho'\}\delta(p-p'\pm k) \tag{77}$$

and

$$-\{\delta_{\mu\nu}\delta_{\rho\sigma}-\delta_{\mu\rho}\delta_{\nu\sigma}\}\delta(p-p'\pm k\pm k') \tag{78}$$

in place of (56) and (57).

Hereafter we verify the equivalence. In this case, the typical adjacent meson lines are as follows :

(i) $T_F^{\nu_2}(p)\beta_\mu T_F^{\nu_2}(p')=0,$ (79)

(ii) $T_F^{\nu_3}(p)\beta_\mu T_F^{\nu_3}(p')=0,$ (80)

because of (29). Others are

(iii) $T_F^{\nu_1}(p)\beta_\mu T_F^{\nu_1}(p')$

$$=(i\beta p-\varkappa)R\frac{-1/\varkappa}{p^2+\varkappa^2}\delta_{\lambda\nu}R_{\lambda\nu}(i\beta p-\varkappa)\delta_\mu(i\beta p'-\varkappa)\delta_{\rho\sigma}R_{\rho\sigma}\times$$

$$\times\frac{-1/\varkappa}{p'^2+\varkappa^2}R(i\beta p'-\varkappa)$$

$$= (i\beta p - \varkappa) R \frac{-1/\varkappa}{p^2+\varkappa^2} \delta_{\lambda\nu}\delta_{\rho\sigma}(-i\varkappa) R_{\lambda\nu}(\beta p\cdot\beta_\mu - \beta_\mu\cdot\beta p') R_{\rho\sigma} \times$$

$$\times \frac{-1/\varkappa}{p'^2+\varkappa^2} R(i\beta p' - \varkappa)$$

$$= (i\beta p - \varkappa) R \frac{-1/\varkappa}{p^2+\varkappa^2} i\{\delta_{\lambda\rho}(p_\mu - p_\mu') - \delta_{\mu\lambda}p_\rho + \delta_{\mu\rho}p_\lambda'\}\delta_{\rho\sigma} \times$$

$$\times \frac{1}{p'^2+\varkappa^2} R_{\lambda\sigma}(i\beta p' - \varkappa). \tag{81}$$

(iv) $T_F^{\nu_1}(p)\beta_\mu T_F^{\nu_3}(p')$

$$= (i\beta p - \varkappa) R \frac{-1/\varkappa}{p^2+\varkappa^2} \delta_{\lambda\nu} R_{\lambda\nu}(i\beta p - \varkappa)\beta_\mu\left(-\frac{1}{\varkappa}\right) R_{\rho\sigma} p_\rho' p_\sigma' \frac{-1/\varkappa}{p'^2+\varkappa^2}$$

$$= (i\beta p - \varkappa) R \frac{-1/\varkappa}{p^2+\varkappa^2} i\delta_{\lambda\nu}(\delta_{\rho\nu}p_\mu - \delta_{\mu\nu}p_\rho)\left(-\frac{1}{\varkappa}\right)^2 p_\rho' p_\sigma' R_{\lambda\sigma}\frac{1}{p'^2+\varkappa^2}$$

$$= (i\beta p - \varkappa) R \frac{-1/\varkappa}{p^2+\varkappa^2} i\{\delta_{\lambda\rho}(p_\mu - p_\mu') - \delta_{\mu\lambda}p_\rho + \delta_{\mu\rho}p_\lambda'\}\left(\frac{1}{\varkappa^2} p_\rho' p_\sigma'\right) \times$$

$$\times \frac{1}{p'^2+\varkappa^2} R_{\lambda\sigma}. \tag{82}$$

(v) $\int dq\, T_{F1}^{\nu_1}(p)\beta_\mu \delta(p - q \pm k)\, T_F^{\nu_2}(q)\beta_\nu \delta(q - p' \pm k')\, T_F^{\nu_3}(p')$

$$= (i\beta p - \varkappa) R \frac{-1/\varkappa}{p^2+\varkappa^2} \delta(p - p' \pm k \pm k')\delta_{\lambda\alpha} R_{\lambda\alpha}(i\beta p' - \varkappa) \times$$

$$\times \beta_\mu\left(-\frac{1}{\varkappa}\right)\frac{1}{2}\beta_\tau\delta_{\varepsilon\tau} R_{\varepsilon\tau}\beta_\tau\beta_\nu(i\beta p' - \varkappa)\delta_{\rho\sigma} R_{\rho\sigma}\frac{-1/\varkappa}{p'^2+\varkappa^2} R(i\beta p - \varkappa)$$

$$= (i\beta p - \varkappa) R \frac{-1/\varkappa}{p^2+\varkappa^2} \delta(p - p' \pm k \pm k')\,\delta_{\lambda\alpha}\delta_{\varepsilon\tau}\delta_{\rho\sigma}(-\varkappa^2)\frac{1}{2} \times$$

$$\times R_{\lambda\alpha}\beta_\mu\beta_\tau R_{\varepsilon\tau}\beta_\tau\beta_\nu R_{\rho\sigma}\frac{(-1/\varkappa)^2}{p'^2+\varkappa^2} R(i\beta p' - \varkappa)$$

$$= (i\beta p - \varkappa) R \frac{-1/\varkappa}{p^2+\varkappa^2} \delta(p - p' \pm k \pm k')\, i^2\{-(\delta_{\mu\nu}\delta_{\rho\lambda} - \delta_{\mu\rho}\delta_{\nu\lambda})\} \times$$

$$\times \delta_{\rho\sigma}\frac{1}{p'^2+\varkappa^2} R_{\lambda\alpha}(i\beta p' - \varkappa). \tag{83}$$

(iv) $\int dq\, T_F^{\nu_1}(p)\beta_\mu \delta(p - q \pm k)\, T_F^{\nu_2}(q)\beta_\nu \delta(q - p' \pm k')\, T_F^{\nu_3}(p')$

$$= (i\beta p - \varkappa) R \frac{-1/\varkappa}{p^2+\varkappa^2} \delta(p - p' \pm k \pm k')\,\delta_{\lambda\alpha} R_{\lambda\alpha}(i\beta p - \varkappa)\beta_\mu \times$$

$$\times\left(-\frac{1}{\varkappa}\right)\frac{1}{2}\beta_\tau\delta_{\varepsilon\tau} R_{\varepsilon\tau}\beta_\tau\beta_\nu\left(-\frac{1}{\varkappa}\right) R_{\rho\sigma} p_\rho' p_\sigma' \frac{-1/\varkappa}{p'^2+\varkappa^2}$$

$$= (i\beta p - \varkappa) R \frac{-1/\varkappa}{p^2+\varkappa^2} \delta(p - p' \pm k \pm k') \delta_{\lambda\alpha} \delta_{\varepsilon\tau}(-\varkappa) \times$$

$$\times \frac{1}{2} R_{\lambda\alpha} \beta_\mu \beta_\tau R_{\varepsilon\tau} \beta_\tau \beta_\nu R_{\rho\sigma} \left(-\frac{1}{\varkappa}\right)^2 p_\rho' p_\sigma' \frac{-1/\varkappa}{p'^2+\varkappa^2}$$

$$= (i\beta p - \varkappa) R \frac{-1/\varkappa}{p^2+\varkappa^2} \delta(p - p' \pm k \pm k') i^2 \{ -(\delta_{\mu\nu}\delta_{\rho\lambda} - \delta_{\mu\rho}\delta_{\nu\lambda}) \} \times$$

$$\times \left(\frac{1}{\varkappa^2} p_\rho' p_\sigma'\right) \frac{1}{p'^2+\varkappa^2} R_{\lambda\sigma} \,. \qquad (84)$$

In these calculations, (25), (28), (29) and (37) are used. For brevity, δ-functions of vertices are omitted in (79), (80), (81) and (82). In (82) the last reformation is due to the identity $(\delta_{\mu\rho} p_\lambda' - \delta_{\rho\lambda} p_\mu') p_\rho' = 0$. In view of Stueckelberg's formulation of meson, this term comes from the B field part of $\chi_{\mu\nu} (= \partial_\mu u_\nu - \partial_\nu u_\mu)$, i.e., $\partial_\mu(\partial_\nu B) - \partial_\nu(\partial_\mu B)$, which is identically equal to zero. (81) and (82) are combined to

$$\cdots i \{\delta_{\lambda\rho}(p_\mu - p_\mu') - \delta_{\mu\lambda} p_\rho + \delta_{\mu\rho} p_\lambda'\} \delta_{\rho\sigma} \frac{1}{p'^2+\varkappa^2} R_{\lambda\sigma} \cdots$$

$$+ \cdots i \{\delta_{\lambda\rho}(p_\mu - p_\mu') - \delta_{\mu\lambda} p_\rho + \delta_{\mu\rho} p_\lambda'\} \frac{1}{\varkappa^2} p_\rho' p_\sigma' \frac{1}{p'^2+\varkappa^2} R_{\lambda\sigma} \cdots$$

$$= \cdots i \{\delta_{\lambda\rho}(p_\mu - p_\mu') - \delta_{\mu\lambda} p_\rho + \delta_{\mu\rho} p_\lambda'\} \frac{\delta_{\rho\sigma} + 1/\varkappa^2 \cdot p_\rho' p_\sigma'}{p'^2+k^2} R_{\lambda\sigma} \cdots \qquad (95)$$

Omitted outer parts are not same for both terms, but are similarly combined with the corresponding terms and give the same factors. Similarly (83) and (84) are combined to

$$\cdots i^2 \{ -(\delta_{\mu\nu}\delta_{\rho\lambda} - \delta_{\mu\rho}\delta_{\nu\lambda}) \delta(p - p' \pm k \pm k') \} \frac{\delta_{\rho\sigma} + 1/\varkappa^2 \cdot p_\rho' p_\sigma'}{p'^2+\varkappa^2} R_{\lambda\sigma} \cdots \,. \qquad (86)$$

Thus the factor $\{\delta_{\lambda\rho}(p_\mu - p_\mu') - \delta_{\mu\lambda} p_\rho + \delta_{\mu\rho} p_\lambda'\} \delta(p - p' \pm k)$ and $-(\delta_{\mu\nu}\delta_{\rho\lambda} - \delta_{\mu\rho}\delta_{\nu\lambda}) \times \delta(p - p' \pm k \pm k')$ in (85) and (86) are just the 3-vertex and 4-vertex factors (77) and (78), respectively. Also, the factor $\frac{\delta_{\rho\sigma} + 1/\varkappa^2 \cdot p_\rho' p_\sigma'}{p'^2+\varkappa^2}$ is just equal to the vector meson propagation function (76) of wave formalism. For an open polygon, the end meson line is the external one, which we can treat as in the scalar case. Thus, there remain finally the outermost meson functions which give (considering that $R R_{\rho\sigma} = R_{\rho\sigma}$ deduced from (35))

$$\bar{\psi}(p) R \cdots R_{\rho\sigma} \psi(q) = \varkappa u_\rho^*(p) \cdots u_\sigma(q) \qquad (87)$$

using relations (39). When the connected meson line is the closed loop, then remains

$$S p R_{\rho\sigma} = \delta_{\rho\sigma} \,. \qquad (88)$$

This Kronecker's δ guarantees that the connected meson lines are closed. The difference of the i-factors and the sign involved in (53) and (59), and also the weight factor (58)

are explained as in the scalar case, too. Thus, the S matrix of vector electrodynamics in β-formslism is also equivalent with that in wave formalism, completely.

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References

1) M. Neuman and W. H. Furry, Phys. Rev. **76** (1949), 1677.
R. G. Moorhouse, Phys. Rev. **76** (1949), 1991.
2) T. Kinoshita, Prog. Theor. Phys. **5** (1950), 473.
T. Kinoshita and Y. Nambu, Prog. Theor. Phys. **5** (1950), 749.
3) D. C. Peaslee, Phys. Rev. **81** (1951), 94.
4) A. H. Wilson, Proc. Camb. Phil. Soc. **36** (1940), 363.
5) Harish-Chandra, Proc. Roy. Soc. **186** (1946), 502.
6) Vachaspati, Proc. Phys. Soc. **63** (1950), 1015; **64** (1951), 659.
7) A. Klein, Phys. Rev. **82** (1951), 639.
8) R. C. Majumdar, A. S. Apte and M. K. Sundaresan, Prog. Theor. Phys. **6** (1951), 737.
9) R. J. Duffin, Phys. Rev. **54** (1938), 1114.
10) I. Fujiwara, Prog. Theor. Phys. (to be published).
11) D. C. Peaslee, Prog. Theor. Phys. **6** (1951), 639.
12) K. V. Roberts, Phys. Rev. **83** (1951), 188.
13) Z. Koba, Prog. Theor. Phys. **5** (1950), 696.
K. Nishijima, Prog. Theor. Phys. **5** (1950), 813.
P. T. Matthews, Phys. Rev. **76** (1949), 684.
14) F. Rohrlich, Phys. Rev. **80** (1950), 666.
15) A. Salam, Proc. Roy. Soc. **211** (1952), 276.
16) N. Kemmer, Proc. Roy. Soc. **173** (1939), 91.
17) S. Kanesawa and S. Tomonaga, Prog. Theor. Phys. **3** (1948), 101.

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Calculation of Heteronuclear Molecular Integrals

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Reduction formulas and numerical tables of heteronuclear molecular integrals and auxiliary integrals are given for several values of parameters.

Introduction

The electronic states of the ethylene molecule was discussed by one of the present authors.[1] To obtain energy values it was necessary to have numerical tables for heteronuclear molecular integrals. Homonuclear integrals were evaluated by many authors[2)-5)] for various values of parameters. However, Coulomb and hybrid heteronuclear integrals had not yet been evaluated, but only methods of estimating their approximate values were given by Sklar,[6] Mayer and McCallum,[7] and Mulligan.[8] Therefore we had to derive the reduction formulas and to compute the numerical values for these heteronuclear and related mononuclear molecular integrals involving 2s, $2p\sigma$ and $2p\pi$ orbitals. After carrying out the evaluation we received three papers[9)10)11)] in which the systematic methods of evaluating heteronuclear molecular integrals were discussed. Our method was different and our reduction formulas were not the same as their result. Although our result is neither complete nor systematic we think some of these formulas and numerical tables may be useful for other calculation. For this reason they will be given in what follows.

§ 1. Definition and method

In the present paper atomic $2s$ and $2p$ orbitals are defined as was done by Araki and Watari.[4] The customary p_x and p_y are denoted by ξ and η in order to avoid double super- or subscripts for the sake of printing convenience:

$$\begin{aligned} s&=Nr\ \exp(-\varkappa r/2), \qquad \sigma=N_1 z\ \exp(-\varkappa r/2), \\ \xi&=N_1 x\ \exp(-\varkappa r/2), \qquad \eta=N_1 y\ \exp(-\varkappa r/2) \end{aligned} \tag{1·1}$$

where the molecular axis is chosen as the z-axis, and

$$N=\{\varkappa^5/(96\pi)\}^{1/2}, \qquad N_1=3^{1/2}N \tag{1·2}$$

are normalization constants. Two atoms are distinguished by suffices a and b. If a σ-orbital, for example, belongs to the a-atom we denote the orbital by σ_a. Further if the effective charge of a ξ-orbital, for example, is $\varkappa_0$ we denote the orbital by ξ^0. Two orbitals

π and $\bar{\pi}$ of Araki and Watari[4] are given by

$$\pi = 2^{-1/2}(\xi + i\eta), \qquad \bar{\pi} = 2^{-1/2}(\xi - i\eta). \tag{1·3}$$

All quantities are measured in atomic units throughout the present paper.

The mononuclear, and heteronuclear Coulomb and hybrid integrals are defined as follows

Mononuclear integral

$$M(\varphi\psi,\ \chi\zeta) = \iint \varphi_a(1)\psi_a(1) r_{12}^{-1} \chi_a(2)\zeta_a(2)\, dv_1\, dv_2\,, \tag{1·4}$$

Coulomb integral

$$C(\varphi\psi,\ \chi\zeta) = \iint \varphi_a(1)\psi_a(1) r_{12}^{-1} \chi_b(2)\zeta_b(2)\, dv_1\, dv_2, \tag{1·5}$$

Hybrid integral

$$H(\varphi\psi,\ \chi\zeta) = \iint \varphi_a(1)\psi_b(1) r_{12}^{-1} \chi_b(2)\zeta_b(2)\, dv_1\, dv_2, \tag{1·6}$$

where φ, ψ, χ or ζ stands for one of s, σ, ξ, and η. The first two are in accord with the notaion of Barnett and Coulson[9], and they can be represented by F, D, and L of Araki and Watari[4] as follows:

$$M(\varphi\psi,\chi\zeta) = F_{\varphi\chi\psi\zeta}, \qquad C(\varphi\psi,\chi\zeta) = D_{\varphi\chi\psi\zeta}, \qquad H(\varphi\psi,\chi\zeta) = L_{\psi\zeta\chi\varphi}. \tag{1·7}$$

The relation between the integrsls involving ξ and η and those involving π and $\bar{\pi}$ were given by Araki and Watari[4].

If the potential due to a neutral carbon atom consisting of a $2s$-electron, three $2p$-electrons (σ, ξ and η) and a nucleus of atomic number 4 (perfectly screening by two ls-electrons) is denoted by U, the penetration integrals are defined as follows:

Mononuclear-penetration integral

$$P(\psi) = \int U_a^0(1)\,|\psi_a(1)|^2 dv_1, \tag{1·8}$$

Coulomb-penetration integral

$$Q(\psi) = \int U_a^0(1)\,|\psi_b(1)|^2\, dv_1, \tag{1·9}$$

Hybrid-penetration integral.

$$R(\varphi\psi) = \int U_a^0(1)\varphi_a(1)\psi_b(1)\, dv_1, \tag{1·10}$$

where the superscript o means that the effective charge is $\varkappa_0$ and the subscripts a and b distinguish two atoms as before.

The mononuclear integrals can immediately be calculated in polar coordinates. The Coulomb and hybrid integrals can be calculated in the following way. We first calculate, in polar coordinates, the potential due to the charge distribution of the second electron

and then integrate, in elliptic coordinates, with respect to the first electron. For calculating the potential U in the definition of the penetration integrals we adopt a 2s-orbital with a node which is different from (1·1). The explicit form of U is thus given by[12]

$$U^0 = -(4r)^{-1}[16+12x_0r+4(x_0r)^2+(x_0r)^3]\exp(-x_0r). \tag{1·11}$$

In order to evaluate the above mentioned integrals we use the following auxiliary integrals :

$$A_n(p) = \int_1^\infty x^n \exp(-px)\, dx, \tag{1·12}$$

$$B_n(q) = \int_{-1}^1 x^n \exp(-qx)\, dx, \tag{1·13}$$

$$F_{m,n}(p,q) = \int_1^\infty dx \int_{-1}^1 dy\,(x+y)^{-m}(-y)^n(1-y^2)^{m-1}\exp(-px-qy), \tag{1·14}$$ *

$$J_n(p,q) = \int_1^\infty dx \int_{-1}^1 dy\,(x^2-1)(1-y^2)(x^2-y^2)(x+y)^n \exp(-px-qy), \tag{1·15}$$

$$K_n(p,q) = \int_1^\infty dx \int_{-1}^1 dy\,(x^2-1)(1-y^2)(x^2-y^2)(1+xy)^2(x+y)^{n-2}\exp(-px-qy). \tag{1·16}$$

J_n and K_n can be represented in terms of $A_n(p)$, $B_n(q)$, and $F_{mn}(p,q)$ where the numerical values of $A_n(p)$ and $B_n(q)$ were computed by Kotani, Amemiya, and Simose.[2] The function F_{omo} of Kotani et al is given in terms of A_n, B_n and F_{mn} as follows :

$$F_{omo}(p,q) = \sum_{k=0}^{m}(-1)^k B_k(q) A_{m-k}(p) + F_{1m}(p,q). \tag{1·17}$$

§ 2. Examination of approximate method

We shall examine the approximate method of Sklar[6], Mayer and McCallum,[7] and Mulligan[8] by comparing the approximate values with the exact values obtained in the present paper. They assumed a geometrical mean of two homonuclear integrals corresponding to two different effective charges as an approximate value of a heteronuclear Coulomb integral. As for the hybrid integrals Mulligan[8] assumed

$$H(\xi\xi^0,\xi^0\zeta^0) = \frac{S(\xi,\zeta^0)}{S(\xi^0,\zeta^0)} H(\xi^0\zeta^0,\xi^0\zeta^0) \tag{2·1}$$

where $S(\varphi,\psi)$ is an overlap integral of two orbitals φ and ψ. The values obtained by these approximate methods are compared with our exact values for few examples as follows :

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* We wish to express our sincere thanks to Assistant Professor K. Yano, of Nara Women's University for the valuable suggestion he has given in evaluating this integral.

		$\rho_0=8,\ \rho=6$	$\rho_0=8,\ \rho=4$	$\rho_0=8,\ \rho=2$
$x_0^{-1}C(\xi\xi,\ \xi^0\xi^0)$	exact	0.10240	0.08873	0.0566
	approx.	0.10290	0.09245	0.0705
	error	+0.5%	+4.1%	+24.6%
$x_0^{-1}H(\xi\xi^0,\ \xi^0\xi^0)$	exact	0.05458	0.05567	
	approx.	0.05389	0.05725	
	error	−1.3%	+2.8%	

We see that the error is small when the difference between effective charges is not large but it becomes larger with the difference between effective charges.

Reduction formulas

Abbreviation : $\lambda=x/x_0$, $\rho=xR$, $\rho_0=x_0R$, $R=$internuclear distance, and s^0, σ^0, ξ^0 and η^0 mean that the effective charge in these orbitals is x_0.

(A) Mononuclear integrals

$$M(\xi\xi,\ \xi^0\xi^0)=(x_0/20)[5\lambda+4\lambda^3-(\lambda^5/(1+\lambda)^7)\{45+45(1+\lambda)+31(1+\lambda)^2+17(1+\lambda)^3+8(1+\lambda)^4+4(1+\lambda)^5\}],$$

$$M(\eta\eta,\ \xi^0\xi^0)=(x_0/20)[5\lambda-2\lambda^3-(\lambda^5/(1+\lambda)^7)\{15+15(1+\lambda)+7(1+\lambda)^2-(1+\lambda)^3-4(1+\lambda)^4-2(1+\lambda)^5\}],$$

$$M(\xi\eta,\ \xi^0\eta^0)=[M(\xi\xi,\ \xi^0\xi^0)-M(\eta\eta,\ \xi^0\xi^0)]/2.$$

(B) Coulomb and hybrid integrals

$$\left.\begin{matrix}C(\xi\xi,\ s^0s^0)\\ H(\xi\xi^0,\ s^0s^0)\\ H(\xi\xi,\ s^0s^0)\end{matrix}\right\}=(x_0/24)Z\left\{\begin{matrix}(\rho/4)^5\\ (\rho\rho_0)^{5/2}/4^5,\\ (\rho/4)^5\end{matrix}\right.$$

$$\left.\begin{matrix}C(\xi\xi,\ \sigma^0\sigma^0)\\ H(\xi\xi^0,\ \sigma^0\sigma^0)\\ H(\xi\xi,\ \sigma^0\sigma^0)\end{matrix}\right\}=\left\{\begin{matrix}C(\xi\xi,\ s^0s^0)\\ H(\xi\xi^0,\ s^0s^0)+(x_0/24)(3Y-X)\\ H(\xi\xi,\ s^0s^0)\end{matrix}\right\}\left\{\begin{matrix}(\rho/4)^5\\ (\rho\rho_0)^{5/2}/4^5,\\ (\rho/4)^5\end{matrix}\right.$$

$$\left.\begin{matrix}C(\xi\eta,\ \xi^0\eta^0)\\ H(\xi\eta^0,\ \xi^0\eta^0)\\ H(\xi\eta,\ \xi^0\eta^0)\end{matrix}\right\}=(x_0/32)(X-Y)\left\{\begin{matrix}(\rho/4)^5\\ (\rho\rho_0)^{5/2}/4^5,\\ (\rho/4)^5\end{matrix}\right.$$

$$\left.\begin{matrix}C(\xi\xi,\ \xi^0\xi^0)\\ H(\xi\xi^0,\ \xi^0\xi^0)\\ H(\xi\xi,\ \xi^0\xi^0)\end{matrix}\right\}=(3/2)\left\{\begin{matrix}C(\xi\xi,\ s^0s^0)\\ H(\xi\xi^0,\ s^0s^0)\\ H(\xi\xi,\ s^0s^0)\end{matrix}\right.-(1/2)\left\{\begin{matrix}C(\xi\xi,\ \sigma^0\sigma^0)\\ H(\xi\xi^0,\ \sigma^0\sigma^0)\\ H(\xi\xi,\ \sigma^0\sigma^0)\end{matrix}\right.+\left\{\begin{matrix}C((\xi\eta,\ \xi^0\eta^0)\\ H(\xi\eta^0,\ \xi^0\eta^0),\\ H(\xi\eta,\ \xi^0\eta^0)\end{matrix}\right.$$

$$\left.\begin{matrix}C(\eta\eta,\ \xi^0\xi^0)\\ H(\eta\eta^0,\ \xi^0\xi^0)\\ H(\eta\eta,\ \xi^0\xi^0)\end{matrix}\right\}=\left\{\begin{matrix}C(\xi\xi,\ \xi^0\xi^0)\\ H(\xi\xi^0,\ \xi^0\xi^0)-2\\ H(\xi\xi,\ \xi^0\xi^0)\end{matrix}\right\}\left\{\begin{matrix}C(\xi\eta,\ \xi^0\eta^0)\\ H(\xi\eta^0,\ \xi^0\eta^0),\\ H(\xi\eta,\ \xi^0\eta^0)\end{matrix}\right.$$

$$X=(1152/\rho_0^3)J_{-3}(p',q')-[(\rho_0/2)^2J_2(p,q)+3\rho_0J_1(p,q)+24J_0(p,q)$$
$$+(144/\rho_0)J_{-1}(p,q)+(576/\rho_0^2)J_{-2}(p,q)+(1152/\rho_0^3)J_{-3}(p,q)],$$
$$Y=(1152/\rho_0^3)K_{-3}(p',q')-[(\rho_0/2)^2K_2(p,q)+3\rho_0K_1(p,q)+24K_0(p,q)$$
$$+(144/\rho_0)K_{-1}(p,q)+(576/\rho_0^2)K_{-2}(p,q)+(1152/\rho_0^3)J_{-3}(p,q)],$$
$$Z=(48/\rho_0)J_{-1}(p',q')-[(\rho_0/2)^2J_2(p,q)+3\rho_0J_1(p,q)$$
$$+18J_0(p,q)+(48/\rho_0)J_{-1}(p,q)].$$

p, q, p' and q' are given by the following table:

		t'	q'	p	q
$Q(\xi)$,	$C(\varphi\psi,\ \chi^0\zeta^0)$	$\rho/2$	$-\rho/2$	$(\rho_0+\rho)/2$	$(\rho_0-\rho)/2$
$R(\xi^0\xi)$,	$H(\varphi\psi^0,\ \chi^0\zeta^0)$	$(\rho_0+\rho)/4$	$(\rho_0-\rho)/4$	$(3\rho_0+\rho)/4$	$(3\rho_0-\rho)/4$
$R(\xi\xi)$,	$H(\varphi\psi,\ \chi^0\zeta^0)$	$\rho/2$	0	$(\rho_0+\rho)/2$	$\rho_0/2$

(C) Penetration integrals

$$P(\xi)=\varkappa_0(\lambda/(1+\lambda))^5[(1+\lambda)+3+5(1+\lambda)^{-1}+(15/2)(1+\lambda)^{-2}],$$

$$\left.\begin{matrix}Q(\xi)\\R(\xi^0\xi)\\R(\xi\xi)\end{matrix}\right\}=\tfrac{1}{4}[(\rho_0/4)^2J_2(p,q)+(\rho_0/2)J_1(p,q)+3J_0(p,q)$$
$$+(8/\rho_0)J_{-1}(p,q)]\left\{\begin{matrix}\varkappa_0(\rho/4)^5\\ \varkappa_0(\rho\rho_0)^{5/2}/4^5\\ \varkappa_0(\rho/4)^5\end{matrix}\right.$$

(D) Auxiliary integrals $J_n(p,q)$

$$A_n=A_n(p),\ B_n=B_n(q),\ F_{mn}=F_{mn}(p,q),$$
$$J_2(p,q)=A_6(B_0-B_2)-2A_5(B_3-B_1)-A_4(B_0-B_2)+2A_3(B_5-B_1)$$
$$-A_2(B_4-B_6)-2A_1(B_3-B_5)+A_0(B_4-B_6),$$
$$J_1(p,q)=A_5(B_0-B_2)-A_4(B_3-B_1)-A_3(B_0-B_4)+A_2(B_5-B_1)$$
$$+A_1(B_2-B_4)-A_0(B_5-B_3),$$
$$J_0(p,q)=A_4(B_0-B_2)-A_2(B_0-B_4)+A_0(B_2-B_4),$$
$$J_{-1}(p,q)=A_3(B_0-B_2)+A_2(B_3-B_1)-A_1(B_0-B_2)-A_0(B_3-B_1),$$
$$J_{-2}(p,q)=A_2(B_0-B_2)+2A_1(B_3-B_1)-A_0(B_0-3B_2+2B_4)-2(F_{11}-2F_{13}+F_{15}),$$
$$J_{-3}(p,q)=A_1(B_0-B_2)+3A_0(B_3-B_1)+(-F_{10}+6F_{12}-5F_{14})-2(F_{21}-F_{23}),$$
$$J_{-1}(\rho/2,-\rho/2)=(512/\rho^5)-(3072/\rho^7)$$
$$+2\{A_3(\rho/2)-A_1(\rho/2)\}\{A_2(\rho/2)-A_0(\rho/2)\},$$
$$J_{-3}(\rho/2,-\rho/2)=(128/\rho^5)+(16/3)\{A_1(\rho)-A_4(\rho)\},$$
$$J_{-3}(p,\rho)=(4/3)A_1+(F_{10}-6F_{12}+5F_{14}).$$

(E) Auxiliary integrals $K_n(p,q)$

$$K_2(p,q)=A_6(B_2-B_4)-2A_5(B_3-B_1)+A_4(B_0-2B_2+B_6)+2A_3(B_5-B_1)$$
$$-A_2(B_0-2B_4+B_6)-2A_1(B_5-B_3)+A_0(B_2-B_4),$$

$$K_1(p,q)=A_5(B_2-B_4)-A_4(-2B_1+3B_3-B_5)+A_3(B_0-4B_2+3B_4)$$
$$+A_2(-3B_1+4B_3-B_5)-A_1(B_0-3B_2+2B_4)-A_0(B_3-B_1),$$

$$K_0(p,q)=A_4(B_2-B_4)-A_3(-2B_1+4B_3-2B_5)+A_2(B_0-6B_2+7B_4-2B_6)$$
$$+A_1(-4B_1+10B_3-8B_5+2B_7)-A_0(B_0-7B_2+12B_4-8B_6+2B_8)$$
$$-2(F_{11}-4F_{13}+6F_{15}-4F_{17}+F_{19}),$$

$$K_{-1}(p,q)=A_3(B_2-B_4)-A_2(-2B_1+5B_3-3B_5)$$
$$-A_1(-B_0+8B_2-12B_4+5B_6)+A_0(-5B_1+18B_3-20B_5+7B_7)$$
$$+(-F_{10}+12F_{12}-30F_{14}+28F_{16}-9F_{18})-2(F_{21}-3F_{23}+3F_{25}-F_{27}),$$

$$K_{-2}(p,q)=A_2(B_2-B_4)-A_1(-2B_1+6B_3-4B_5)-A_0(-B_0+10B_2-18B_4+9B_6)$$
$$+2(3F_{11}-14F_{13}+19F_{15}-8F_{17})+(-F_{20}+11F_{22}-19F_{24}+9F_{26})$$
$$+2(-F_{31}+2F_{33}-F_{35}),$$

$$K_{-3}(p,q)=A_1(B_2-B_4)+A_0(2B_1-7B_3+5B_5)$$
$$+(F_{10}-12F_{12}+25F_{14}-14F_{16})+2(3F_{21}-11F_{23}+8F_{25})$$
$$+(-F_{30}+10F_{32}-9F_{34})+2(F_{43}-F_{41}),$$

$$K_{-3}(\rho/2,-\rho/2)=(128/\rho^5)-(3072/\rho^7)+(16/15)\{A_1(\rho)-5A_4(\rho)+4A_6(\rho)\}$$
$$=J_{-3}(\rho/2,-\rho/2)-(3072/\rho^7)-(64/15)\{A_1(\rho)-A_6(\rho)\},$$

$$K_{-1}(p,o)=(4/15)A_3+(4/105)A_1+(F_{10}-12F_{12}+30F_{14}+28F_{16}-9F_{18}),$$

$$K_{-2}(p,o)=(4/15)A_2-(4/105)A_0-2(-3F_{11}+14F_{13}-19F_{15}+8F_{17}),$$

$$K_{-3}(p,o)=(4/15)A_1+(-F_{10}+12F_{12}-25F_{14}+14F_{16}).$$

(F) Auxiliary integrals $F_{mn}(p,q)$

$$B_n=B_n(q),\qquad \delta=p-q>0,\ q>0,$$

$$F_{10}(p,q)=[\log(p/q)-\{-Ei(-2q)\}](e^{-\delta}/\delta)+[-Ei(-2p)](e^{\delta}/\delta),$$

$$F_{1,n}(p,q)=[\log(p/q)-\{-Ei(-2q)\}](e^{-\delta}/\delta)+(-1)^n[-Ei(-2p)](e^{\delta}/\delta)$$
$$-(e^{-p}/\delta)\textstyle\sum_{k=0}^{n-1}(-1)^kB_k(q)+(n/\delta)F_{1,n-1},$$

$$F_{2,n}(p,q)=(-1)^ne^{-p}(B_n-B_{n+1})-p(F_{1,n}-F_{1,n+2}),$$

$$2F_{3,n}(p,q)=(-1)^ne^{-p}(B_n-2B_{n+1}+B_{n+2})-p(F_{2,n}-F_{2,n+2}),$$

$$3F_{4,n}(p,q)=(-1)^ne^{-p}(B_n-3B_{n+1}+3B_{n+2}-B_{n+3})-p(F_{3,n}-F_{3,n+2}),$$

$$F_{1,0}(p,\rho)=(e^{-p}/p)[C+\log(2p)]+(e^{p}/p)[-Ei(2p)],$$

$$F_{1,n}(p,\rho)=(e^{-p}/p)\{C+\log(2p)\}+(-1)^{n}(e^{p}/p)[-Ei(-2p)]$$

$$-(e^{-p}/p)\sum_{k=0}^{n-1}(-1)^{k}B_{k}(0)+(n/p)F_{1,n-1}(p,\rho),$$

$$C=0.57721\ 56649\ 01532\ 86060\ 65120\ 90082\ 40243\ 10421\ \ldots.$$

F_{1n} in the present paper is equal to $(-1)^{n}F_{n}$ in the previous paper[1]. The reduction formula, Eq. (15) in the latter, of F_{n} was misprinted: for $\sum_{k=1}^{n-1}$ read $\sum_{k=0}^{n-1}$

Table 1. Mononuclear integrals

x/x_0	$x_0^{-1}M(\xi\xi,\ \xi^0\xi^0)$	$x_0^{-1}M(\eta\eta,\ \xi^0\xi^0)$	$x_0^{-1}M(\xi\eta,\ \xi^0\eta^0)$	$x_0^{-1}P(\xi)$
1	0.19570 3125	0.17460 9375	0.01054 6875	0.29296 875
0.9	0.18506 82906	0.16022 58801	0.01242 12053	0.22915 48856
0.8	0.17256 66667	0.15440 22134	0 00908 22267	0.17155 26904
0.7	0.15795 05236	0.14192 64185	0.00801 20525	0.12116 85649
0.6	0.14100 51584	0.12758 33845	0.00671 08870	0.07901 27778
0.5	0.12160 49383	0.11117 96982	0.00521 26200	0.04595 33608
0.4	0.09979 98890	0.09258 71509	0.00360 63691	0.02246 29437
0.3	0.07592 83164	0.07181 04501	0.00205 89331	0.00823 58616

Table 2. Coulomb integrals

	ρ / ρ_0	2	4	6	8	10
$x_0^{-1}C(\xi\xi,\ \xi^0\xi^0)$	6	0.073 349 301	0.113 617 881	0.132 415 195		
	8	0.055 568 482	0.087 651 475	0.103 175 483	0.110 869 965	
	10	0.044 607 851	0.070 834 819	0.083 652 448	0.089 964 768	0.093 298 127
$x_0^{-1}G(\xi\xi,\ \sigma^0\sigma^0)$	6	0.072 936	0 116 944 4	0.142 235 8		
	8	0.055 364	0.089 381 3	0.108 706 9	0.119 972 662	
	10	0.044 482	0.071 789 1	0.086 863 6	0.095 332 382	0.100 278 752
$x_0^{-1}C(\xi\xi,\ \xi^0\xi^0)$	6	0.075 329	0.115 355 7	0.130 780 6		
	8	0.056 559	0.088 734 3	0.102 393 5	0.107 950 969	
	10	0.045 172	0.071 530 8	0.083 272 8	0.088 294 622	0.090 591 146
$x_0^{-1}C(\eta\eta,\ \xi^0\xi^0)$	6	0.071 783	0 108 553 5	0.124 229 1		
	8	0 054 782	0.084 838 8	0.098 426 0	0.104 686 264	
	10	0.044 169	0.069 184 7	0.080 821 0	0.086 267 301	0.089 024 482
$x_0^{-1}C(\xi\eta,\ \xi^0\eta^0)$	6	0.001 773	0.003 401 1	0.003 275 8		
	8	0.000 889	0.001 947 8	0.001 983 7	0.001 632 353	
	10	0.000 502	0.001 173 1	0.001 225 9	0.001 013 660	0,000 783 332

Table 3. Hybrid integrals

	ρ / ρ^0	2	4	6	8	10
$x_0^{-1}H(\xi\xi^0, s^0s^0)$	6	0.050 446 63	0.079 620 24	0.073 491 03		
	8	0.029 974 33	0.052 600 52	0.051 283 95	0.041 511 261	
	10	0.019 367 18	0.035 660 08	0.035 680 49	0.029 059 927	0.021 794 099
$x_0^{-1}H(\xi\xi^0, \sigma^0\sigma^0)$	6	0.048 294 6	0.078 795 1	0.073 643 3		
	8		0.051 576 2	0.049 950 5	0.042 047 9	
	10		0.035 833 5	0.035 299 9	0.028 755 7	0.022 240 8
$x_0^{-1}H(\xi\xi^0, \xi^0\xi^0)$	6	0.054 299 1	0.083 916 0	0.076 889 3		
	8		0 055 671 5	0.054 581 5	0.042 997 0	
	10		0.037 053 8	0.037 492 7	0.030 534 8	0.022 387 3
$x_0^{-1}H(\eta\eta^0, \xi^0\xi^0)$	6	0.048 746 1	0.076 149 6	0.069 940 5		
	8		0.050 553 8	0.049 319 9	0.039 489 0	
	10		0.034 092 9	0.034 248 9	0.027 889 3	0.020 754 2
$x_0^{-1}H(\xi\eta^0, \xi^0\eta^0)$	6	0.002 776 5	0.003 883 2	0 003 474 4		
	8		0.002 558 8	0.002 630 8	0.001 754 0	
	10		0.001 480 4	0.001 621 9	0.001 322 7	0.000 816 5
$x_0^{-1}H(\xi\xi, s^0s^0)$	6	0.069 849 17	0.088 834 03	0.073 491 03		
	8	0.053 110 72	0.069 951 48	0.059 686 36	0.041 511 261	
	10	0.042 708 24	0.057 180 20	0.049 619 93	0.034 958 290	0.021 794 099
$x_0^{-1}H(\xi\xi, \sigma^0\sigma^0)$	6	0.068 388	0.088 210	0.073 643 3		
	8		0.069 064	0.059 607 8	0.042 047 9	
	10		0.056 613	0.049 488 4	0.035 258 7	0.022 240 85
$x_0^{-1}H(\xi\xi, \xi^0\xi^0)$	6	0.072 66	0.092 995	0.076 889 3		
	8		0.072 929	0.062 214 2	0.042 997 0	
	10		0.059 097	0.051 437 6	0.036 103 5	0.022 387 30
$x_0^{-1}H(\eta\eta, \xi^0\xi^0)$	6	0.068 50	0.085 297	0.069 940 5		
	8		0.067 862	0.057 237 1	0.039 489 0	
	10		0.055 830	0.047 933 8	0.033 512 7	0.020 754 16
$x_0^{-1}H(\xi\eta, \xi^0\eta^0)$	6	0.002 08	0.003 849	0.003 474 4		
	8		0.002 534	0.002 488 6	0.001 754 0	
	10		0.001 633	0.001 751 9	0.001 295 4	0.000 816 51

Table 4. Penetration integrals

	ρ / ρ_0	2	4	6	8	10
$x_0^{-1}Q(\xi)$	6	0.005 571 714	0.024 903 334	0.038 662 717		
	8	0.001 627 498	0.007 597 687	0.011 409 320	0.012 369 323	
	10	0.000 593 044	0.002 779 805	0.003 952 862	0.003 933 205	0.003 515 328

	ρ_0 \ ρ	2	4	6	8	10
$x_0^{-1}R(\xi^0\xi)$	6	0.030 109 710	0.058 780 195	0.059 965 560		
	8	0.015 579 044	0.031 348 258	0.032 159 178	0.025 691 954	
	10	0.008 241 463	0.018 520 151	0.019 183 531	0.015 109 076	0.010 451 788
$x_0^{-1}R(\xi\xi)$	6	0.007 670 204	0.039 735 279	0.059 965 560		
	8	0.002 476 168	0.015 174 767	0.025 276 216	0.025 691 954	
	10	0.000 975 968	0.006 680 904	0.011 986 213	0.013 000 625	0.010 451 788

Table 5. $J_n(p, q)$

($0.0_5 30185$ means 0.00000 30185)

(p,q)	(10, 0)	(10, 5)	(9.5, 5.5)	(9, 1)	(9, 5)
J_2	0.0_5 30185 67825	0.0_5 51655 989	0.0_4 12728 748	0.0_5 96347 9620	0.0_4 21367 552
J_1	0.0_5 21428 78018	0.0_5 64136 658	0.0_4 16128 741	0.0_5 74362 4048	0.0_4 24244 262
J_0	0.0_5 17094 58689	0.0_5 95210 994	0.0_4 24415 506	0.0_5 66076 4080	0.0_4 34349 422
J_{-1}	0.0_5 16101 84176	0.0_4 17637 1053	0.0_4 46043 086	0.0_5 71138 3337	0.0_4 60565 954
J_{-2}	0.0_5 19510 65963	0.0_4 43559 8951	0.0_3 11548 7478	0.0_5 10062 377	0.0_3 14193 3442
J_{-3}	0.0_5 35619 83004	0.0_3 16166 69419	0.0_3 43379 1866	0.0_5 21557 644	0.0_3 49784 5235

(p,q)	(9, 6)	(8.5, 6.5)	(8, 0)	(8, 2)	(8, 4)
J_2	0.0_4 32718 018	0.0_4 87747 22	0.0_4 44806 25294	0.0_4 38100 70788	0.0_4 58017 1221
J_1	0.0_4 41927 850	0.0_3 10864 543	0.0_4 29972 69035	0.0_4 31833 42889	0.0_4 59827 8090
J_0	0.0_4 64172 765	0.0_3 17280 747	0.0_3 22517 05531	0.0_4 31122 38662	0.0_4 73331 0631
J_{-1}	0.0_3 12225 6447	0.0_3 33004 730	0.0_4 19874 41349	0.0_4 37347 23389	0.0_3 11150 06571
J_{-2}	0.0_3 30937 4227	0.0_3 83722 994	0.0_4 22278 8742	0.0_4 59187 339	0.0_3 22476 8621
J_{-3}	0.0_2 11703 23632	0.0_2 31737 5437	0.0_4 36682 988	0.0_3 14073 9031	0.0_3 67699 974

(p,q)	(8, 5)	(8, 7)	(7.5, 4.5)	(7, 1)	(7, 3)
J_2	0.0_4 85980 116	0.0_3 24570 431	0.0_3 14672 0577	0.0_3 16403 2575	0.0_3 19371 99258
J_1	0.0_4 96485 282	0.0_3 20540 384	0.0_3 15313 6078	0.0_3 11164 19910	0.0_3 17072 79089
J_0	0.0_3 12903 7932	0.0_3 47677 946	0.0_3 19018 63936	0.0_4 95330 7037	0.0_3 17767 05117
J_{-1}	0.0_3 21439 4271	0.0_3 90584 900	0.0_3 29302 64556	0.0_4 93771 45426	0.0_3 22800 49400
J_{-2}	0.0_3 47236 632		0.0_3 59795 2791	0.0_3 11959 9855	0.0_3 38600 616
J_{-3}	0.0_2 15535 8990		0.0_2 18195 3646	0.0_3 22524 2326	0.0_3 97282 658

(p,q)	(7, 4)	(7, 5)	(6.5, 5.5)	(6, 0)	(6, 2)
J_2	0.0_3 26069 5842	0.0_3 39386 1145	0.0_2 11249 1880	0.0_3 88779 4504	0.0_3 79441 3399
J_1	0.0_3 25192 1517	0.0_3 41093 6143	0.0_2 11574 5132	0.0_3 53689 2961	0.0_3 58847 8547
J_0	0.0_3 28909 4742	0.0_3 51104 9503	0.0_2 14234 1731	0.0_3 36518 2420	0.0_3 50938 5200
J_{-1}	0.0_3 41080 1444	0.0_3 78930 3818	0.0_2 21793 1145	0.0_3 29071 7148	0.0_3 53796 3983
J_{-2}	0.0_3 77185 8990	0.0_2 16153 3450		0.0_3 29024 1767	0.0_3 74212 6733
J_{-3}	0.0_2 21595 4406	0.0_2 49289 4798		0.0_3 41455 3034	0.0_2 15115 2927

(p, q)	(6, 3)	(6, 4)	(6, 5)	(5.5, 3.5)	(5, 1)
J_2	0.0_3 95169 256	0.0_2 13156 6956	0.0_2 20252 638	0.0_2 25903 184	0.0_2 42431 503
J_1	0.0_3 77642 456	0.0_2 11615 2828	0.0_2 19200 371	0.0_2 20959 778	0.0_2 25980 143
J_0	0.0_3 74785 947	0.0_2 12234 3817	0.0_2 21741 878	0.0_2 20114 433	0.0_2 18320 831
J_{-1}	0.0_3 88690 416	0.0_2 15956 6156	0.0_2 30629 291	0.0_2 23850 830	0.0_2 15494 649
J_{-2}	0.0_2 13833 8952	0.0_2 27496 4753		0.0_2 37285 265	0.0_2 16800 115
J_{-3}	$0\,0_2$ 31981 9003	0.0_2 70453 2026		0.0_2 86484 966	0.0_2 26409 911

(p, q)	(5, 3)	(5, 4)	(4, 2)	(4, 3)
J_2	0.0_2 54704 163	0.0_2 77452 479	0.0 31470 684	0.0 40038 923
J_1	0.0_2 40108 250	0.0_2 60995 435	0.0 18419 447	0.0 25187 838
J_0	0.0_2 34789 236	0.0_2 57271 363	0.0 12672 143	0.0 18843 460
J_{-1}	0.0_2 37181 974	0.0_2 66767 959	0.0 10658 267	0.0 17448 799
J_{-2}	0.0_2 52240 196	0.0 10307 056	0.0 11678 838	0.0 21317 802
J_{-3}	0.0 10859 023	0.0 23699 008	0.0 18750 581	0.0 38638 432

Table 6. $K_n(p, q)$

(p, q)	(10, 0)	(10, 5)	(9.5, 5.5)	(9, 1)	(9, 5)
K_2	0.0_5 21666 4722	0.0_5 17237 429	0.0_5 37046 14	0.0_5 59058 73	0.0_5 61431 83
K_1	0.0_5 14590 9321	0.0_5 19525 638	0.0_5 43789 30	0.0_5 42338 46	0.0_5 67831 09
K_0	0.0_5 10777 5340	0.0_5 26370 903	0.0_5 63817 81	0.0_5 33970 52	0.0_5 89217 81
K_{-1}	0.0_6 90426 86	0.0_5 46826 1	0.0_4 10898 83	0.0_5 32114 23	0.0_4 14625 961
K_{-2}	0.0_6 91834 61	0.0_5 95394 3	0.0_4 23820 02	0.0_5 37553 71	0.0_4 32044 160
K_{-3}	0.0_5 12909 0	0.0_4 35899 7	0.0_3 10082 908	0.0_5 61324 80	0.0_3 10616 8849

(p, q)	(9, 6)	(8, 0)	(8, 2)	(8, 4)	(8, 5)
K_2	0.0_5 83544 372	0.0_4 29548 2726	0.0_4 18496 038	0.0_4 18824 189	0.0_4 23089 58
K_1	0.0_4 10196 9622	0.0_4 18714 1627	0.0_4 14154 032	0.0_4 17965 04	0.0_4 24529 74
K_0	0.0_4 14886 599	0.0_4 13001 3996	0.0_4 12403 127	0.0_4 20269 0	0.0_4 29875 62
K_{-1}	0.0_4 27140 401	0.0_4 10238 4439	0.0_4 13023 736	0.0_4 28311 1	0.0_4 48937 67
K_{-2}	0.0_4 66070 12	0.0_5 97043 205	0.0_4 17683 294	0.0_4 52582 9	0.0_3 10278 270
K_{-3}	0.0_3 24218 505	0.0_4 12574 567	0.0_4 35664 901	0.0_3 14735 9	0.0_3 32481 233

(p, q)	(7.5, 4.5)	(7, 1)	(7, 3)	(7, 4)	(7, 5)
K_2	0.0_4 40575 58	0.0_4 87348 6805	0.0_4 68504 83	0.0_4 74456 0	0.0_4 93997 76
K_1	0.0_4 39985 15	0.0_4 57793 5716	0.0_4 55834 42	0.0_4 67785 3	0.0_4 94819 39
K_0	0.0_4 46818 64	0.0_4 43364 8683	0.0_4 53179 12	0.0_4 73062 3	0.0_3 12153 03
K_{-1}	0.0_4 68087 54	$0\,0_4$ 35890 6145	0.0_4 61973 56	0.0_4 97475 0	0.0_3 12669 54
K_{-2}	0.0_3 13161 580	0.0_4 45504 998	0.0_4 95050 05	0.0_3 17277 3	0.0_3 47888 76
K_{-3}	0.0_3 38339 791	0.0_4 50462 904	0.0_3 21841 756	0.0_3 45847 1	0.0_3 72444 12

(p, q)	(6, 0)	(6, 2)	(6, 3)	(6, 4)	(5.5, 3.5)
K_2	0.0_3 51143 997	0.0_3 30792 418	0.0_3 29214 423	0.0_3 32598 1	0.0_3 65985 923
K_1	0.0_3 29343 802	0.0_3 21222 232	0.0_3 22419 313	0.0_3 27832 6	0.0_3 51383 006
K_0	0.0_3 18528 436	0.0_3 16817 025	0.0_3 20165 394	0.0_3 28192	0.0_3 47312 43
K_{-1}	0.0_3 13268 805	0.0_3 16013 927	0.0_3 22224 252	0.0_3 35398	0.0_3 47768 4
K_{-2}	0.0_3 11396 293	0.0_3 19690 808	0.0_3 32198 787	0.0_3 5874	0.0_3 80680 8
K_{-3}	0.0_3 13221 32	0.0_3 35667 61	0.0_3 69558 059	0.0_2 14611	0.0_2 18051 66
(p, q)	(5, 1)	(5, 3)	(4, 2)	(4, 3)	
K_2	0.0_2 17963 383	0.0_2 14297 232	0.0_2 86800 921	0.0_2 89081 810	
K_1	0.0_2 10367 906	0.0_2 10086 466	0.0_2 49067 975	0.0_2 55256 490	
K_0	0.0_3 67634 61	0.0_3 83794	0.0_3 32333 838	0.0_2 4092	
K_{-1}	0.0_3 51734 83	0.0_3 85514	0.0_2 25846 20	0.0_2 5604	
K_{-2}	0.0_3 49511 36	0.0_2 11476 9	0.0_2 26869 05	0.0_2 5961	
K_{-3}	0.0_3 67364 92	0.0_2 14892 7	0.0_2 41569 00	0.0 13043	

Table 7. $J_n(p, q)$ and $K_n(p, q)$ for special values of parameters

(p, q)	(5, −5)	(4, −4)	(3, −3)	(2, −2)	(1, −1)
J_{-1}	0.0_2 48139 99430	0.0 14185 54527	0.0 55631 33135	0.35714 43699	7.1575 51722
J_{-3}	0.0_2 12691 91185	0.0_2 37686 57907	0.0 14339 17508	0.07692 14479	0.75195 32022
K_{-3}	0.0_3 98066 29288	0.0_2 25615 80932	0.0_2 79623 20407	0.03174 92251	0.21006 89611
(p, q)	(5, 0)	(4, 0)	(3, 0)	(2, 0)	(1, 0)
J_{-1}	0.0_2 12361 88676	0.0_2 59144 25057	0.0 34420 68924	0.29322 64470	6.86708 2902
J_{-3}	0.0_2 14734 6098	0.0_2 55597 7062	0.0 23094 1369	0.11492 0553	0.91254 219
K_{-3}	0.0_3 44912 3459	0.0_2 16050 788	0.0_2 62364 39	0.028509 5	0.20278
(p, q)	(4.5, 0.5)	(4, 1)	(3.5, 1.5)	(3, 2)	
J_{-1}	0.0_2 29037 00303	0.0_2 73465 85959	0.0 20156 85675	0.060689 35621	
J_{-3}	0.0_2 37209 11041	0.0_2 97202 46443	0.0 26244 03348		
K_{-3}	0.0_3 95552 3271	0.0_2 23503 83411	0.0_2 65066 3017		
(p, q)	(3.5, 0.5)	(3, 1)	(2.5, 1.5)		
J_{-1}	0.0 15026 85281	0.0 42210 67459	0.13397 64673		
J_{-3}	0.0 14405 1675	0.0 39024 3123			
K_{-3}	0.0_2 34129 078	0.0_2 88806 372			
(p, q)	(2.5, 0.5)	(2, 1)			
J_{-1}	0.1 01220 4230	0.3 52670 8883			
J_{-3}	0.0 63072 34946	0.1 85450 4492			
K_{-3}	0.0 14905 69920	0.0 36898 404			

Table 8. $F_{mn}(p, q)$

$F_{1n}(p, q)$

n \ p	10	8	6
0	0.0_4 164378 00406 5	0.0_3 14294 114952	0.0_2 129698 57789
1	0.0_5 85683 10771 2	0.0_4 71994 38285	0.0_3 62300 85763
2	,, 90714 76608 4	,, 77074 08825	67840 45788
3	,, 66193 11729 5	,, 55074 30326	47062 97086
4	,, 69788 77161 7	,, 58657 42518	50907 12841
5	,, 55713 10136 6	,, 46059 27952	39040 32966
6	,, 58579 41360 4	,, 48891 60180	42047 12967
7	,, 48852 89658 5	,, 40197 73222	33869 12543
8	,, 51262 46155 8	,, 42564 06624	36362 05209
9	,, 43894 64918 3	35983 74880	30176 65532

n \ p	5	4	3
0	0.0_2 40041 78753 2	0.01 26787 11843	0.0 41725 59212 5
1	18630 59721 3	0.00 56623 33696	17621 11099
2	20542 23842 0	63520 59247	20281 62053
3	13963 61769 0	42040 93687	12930 40783
4	15276 96435 5	46723 79603	14710 96400
5	11524 88139 4	34489 59869	10528 78485
6	12545 57027 7	38101 61833	11889 71415
7	9961 45999 4	29680 0867	9011 55232
8	10803 79316 0	32644 7945	10121 3251
9	8849 84618 2	26277 6872	7944 9302

n \ p	2	1
0	0.1 46829 01624	0. 60026 57432
1	0.0 56982 3942	19892 19648
2	68476 1272	26235 05905
3	41170 3157	14045 4932
4	48722 603	18107 363
5	33195 576	11161 95
6	38901 64	14181 73
7	28211 21	9386 4
8	32826 2	11791
9	24735 9	806

(p,q)	(10, 5)	(9.5, 5.5)	(9 .1)
F_{10}	0.0_3 93407 51105 91181	0.0_2 25025 71711 39515	0.0_4 90384 74521 83893 348
F_{11}	85138 15693 956	22956 91838 39	64826 1199 107
F_{12}	78949 31071 96	21367 25938 10	58981 4548 86
F_{13}	73937 93753 5	20066 02237 70	50738 21774 01
F_{14}	69761 22440 7	18971 14507 18	47653 95944 54
F_{15}	66187 45739 0	18028 75824 25	42948 66696 54
F_{16}	63082 81164 1	17205 53795 88	40972 63936 77
F_{17}	60345 33732 3	16476 86724 21	37771 58627 86
F_{18}	57908 65880 6	15825 74602 79	36375 29245 48
F_{19}	55718 56677	15238 69889 32	33994 80651 43
F_{20}	0.0_3 97985 31217 70	0.0_2 25811 31923 64	0.0_4 98232 95009 2
F_{21}	87439 32407	23176 13299 12	72471 71907 7
F_{22}	79535 00470	21171 62404 00	61989 13509 6
F_{23}	73205 78915	19548 99447 59	53535 87998 6
F_{24}	67980 93037	18197 62082 49	48057 81075 5
F_{25}	63562 95912	17047 63995 07	43361 59766 1
F_{26}	59767 19007	16053 53286 25	39883 34152 2
F_{27}	56464 3950	15183 02262 07	36792 37675 5
F_{30}	0.0_21 28752 8794	0.0_2 33555 10419 5	0.0_31 26965 53065 8
F_{31}	1 14261 0184	30058 26956 9	0.0_4 96388 44313 9
F_{32}	1 03292 8575	27292 34159 4	81098 25868 5
F_{33}	94523 6742	25055 51208 2	70131 49374 4
F_{34}	87315 9074	23196 32855 5	62287 39610 2
F_{35}	81253 619	21619 14796 3	56045 89971 6
F_{41}	0.0_21 65203 467	0.0_2 43295 29087 9	0.0_3 138155 10999 4
F_{43}	1 36508 10	35996 64192 4	101068 73248 5

(J,J')	(9, 5)	(9, 6)	(8.5, 6.5)
F_{10}	0.0_2 26914 14008 99636	0.0_2 67289 70514 94663	0.0 18152 78885 038125
F_{11}	24485 05205 440	62060 18677 92	16818 78336 13583
F_{12}	22672 50796 54	57954 08356 25	15752 35677 1029
F_{13}	21207 44164 35	54558 54483 81	14862 11867 3185
F_{14}	19988 50761 67	51677 67137 42	14101 24159 500
F_{15}	18946 84869 41	49184 05976 58	13439 15220 523
F_{16}	18043 10380 43	46995 04044 28	12855 35270 242
F_{17}	17246 96270 87	45050 38936 12	12334 92525 255
F_{18}	16538 95310 60	43306 89322 06	11866 91241 32
F_{29}	15902 80551 78	41730 95584 58	11442 83603 56
F_{20}	0.0_2 27761 94348 6	0.0_2 68106 64403 66	0.0 18034 75820 69254
F_{21}	24715 33175 1	61562 69389 17	16385 96098 9581
F_{22}	22439 66072 1	56455 33266 42	15078 65932 5852
F_{23}	20622 04944 0	52279 19575 01	13999 85562 018
F_{24}	19124 30652 9	48774 39365 40	13088 16073 686
F_{25}	17859 75861 9	45774 90380 06	12303 78574 960
F_{26}	16773 85601 4	43169 87296 17	11619 62690 94
F_{27}	15828 06537 0	40880 15479 31	11016 16289 22
F_{30}	0.0_2 36124 95658 7	0.0_2 88171 45366 44	0.0 23164 60061 5672
F_{31}	31984 97425 5	79234 51522 30	20924 42676 0605
F_{32}	28862 43105 6	72232 07633 34	19144 48545 6736
F_{33}	26369 85471 9	66514 50294 61	17678 34651 083
F_{34}	24318 80934 8	61727 66162 42	16442 69681 868
F_{35}	22592 35276 9	57644 19716 77	15383 14496 343
F_{41}	$0\,0_2$ 45945 48744 3	0.01 13711 00232 9	0.0 29915 75865 266
F_{43}	37798 16086 8	0.00 95210 29697 1	25210 66831 327

(p,q)	(8, 2)	(8, 4)	(8, 5)
F_{10}	0.0_3 57159 84084 78862	0.0_2 31737 76537	0.0_2 78000 09745 61899
F_{11}	46319 25680 7	28226 95974	70809 36873 09
F_{12}	41426 02453 4	25817 55517	65461 55985 80
F_{13}	37227 69354 1	23917 12265	61148 07724 05
F_{14}	34461 28483 9	22383 00696	57566 03490 48
F_{15}	31915 63083 7	21089 28081	54509 60860 18
F_{16}	30057 31248 4	19987 07844	51861 59665 61
F_{17}	28277 82334 5	19024 06403	49531 68263 2
F_{18}	26914 43134 8	18178 67158	47462 06060 6
F_{19}	25573 41245 4	17423 19972	45604 36384
F_{20}	0.0_3 61170 88098 5	0.0_2 32773 07868	0.0_2 78926 04947 08
F_{21}	48935 10622 5	28475 55176	70078 12466 58
F_{22}	42342 78116 3	25476 37828	63495 94673 42
F_{23}	37404 22518 3	23151 00196	58253 15175 65
F_{24}	33775 06613 9	21283 48020	53943 15140 53
F_{25}	30819 14822 2	19733 64708	50311 37221 9
F_{26}	28443 03947 0	18423 19992	47198 12919 2
F_{27}	26419 87294 6	17265 03800	44490 77493
F_{30}	0.0_3 79042 11263	0.0_2 42357 70278	0.01 01580 99247 63
F_{31}	63740 63137	36655 30702	0.00 89714 40983 72
F_{32}	54709 85268	32591 65800	80799 34229 73
F_{33}	48113 47805	29442 90300	73702 66098 0
F_{34}	43136 11989	26912 02372	67876 62983 2
F_{35}	39156 74727	24818 48174	62982 20961
F_{41}	0.0_3 90890 83669	0.0_2 52311 42697	0.01 27985 21977 3
F_{43}	68727 39290	41978 52155	0.01 04963 12824

(p,q)	(7.5, 4.5)	(7, 1)	(7, 3)
F_{10}	0.0_2 84774 25301	0.0_3 78744 50214 2	0.0_2 38788 11308
F_{11}	76155 00961	55398 64807	33244 74856
F_{12}	69980 03042	50307 13809	29959 48892
F_{13}	65063 60242	42888 72855	27383 53808
F_{14}	61036 33844	40244 46226	25419 78705
F_{15}	57624 79161	36043 60355	23761 07808
F_{16}	54693 33933	34371 91845	22400 14108
F_{17}	52126 05195	31531 04096	21204 40601
F_{18}	49858 77061	30362 52389	20185 36517
F_{19}	47830 26307	28257 21403	19267 3644
F_{20}	0.0_2 85736 01755	0.0_3 82359 9321	0.0_2 40003 62464
F_{21}	75254 50587	59666 9926	33506 72224
F_{22}	67697 77655	50694 9423	29425 54959
F_{23}	61766 95235	43443 7720	26353 08832
F_{24}	56950 84398	38834 1633	23973 37825
F_{25}	52927 35458	34880 5553	22032 03611
F_{26}	49503 99632	31977 3118	20424 45187
F_{27}	46544 51021	29385 4589	19056 17404
F_{30}	0.01 09922 96964	0.0_2 103501 4905	0.0_2 51146 33201
F_{31}	0.0_2 96029 43740	0.0_3 77403 7789	42831 61042
F_{32}	85865 75277	64733 9337	37374 28581
F_{33}	77892 19373	55679 5501	33286 92145
F_{34}	71419 94094	49206 2516	30098 57799
F_{35}	66029 91549	44022 9463	27512 7947
F_{41}	0.01 3650 65662	0.0_2 109597 9404	0.0_2 60613 20216
F_{43}	1 1060 18411	0.0_3 78705 2844	47147 32053

(p,q)	(7, 4)	(7, 5)	(6, 2)
F_{10}	$0\,0_2$ 92869 57371 57	0 0 22768 20705 371	0.0_2 50196 26183
F_{11}	82343 34015	20618 98543	40140 40682
F_{12}	75155 51292	19026 71865	35714 97818
F_{13}	69499 86528	17745 51025	31902 35467
F_{14}	64946 26117	16683 85454	29432 72934
F_{15}	61112 81539	15779 55272	27147 25889
F_{16}	57853 08187	14997 34991	25503 87703
F_{17}	55008 78975	14310 05434	23919 02890
F_{18}	52515 71521	13699 89077	22722 28089
F_{19}	50290 21422	13151 69115	21535 31927
F_{20}	0.0_2 93830 4371	0.0 22530 52888	0.0_2 51318 2463
F_{21}	81223 0656	19944 57345	40472 5684
F_{22}	72475 7738	18029 74866	34764 1074
F_{23}	65716 5675	16509 32865	30508 5206
F_{24}	60304 7140	15262 75309	27416 4300
F_{25}	55824 1647	14214 68476	24907 0325
F_{26}	52043 9590	13314 91086	22905 4857
F_{27}	48795 5617	12525 75169	21205 9695
F_{30}	0.0 11973 68047	0.0 28637 19292	0.0_2 64390 9978
F_{31}	10326 12197	25220 99177	51287 0974
F_{32}	0.0_2 9158 45171	22665 92990	43705 3157
F_{33}	8256 80331	20638 40482	38209 8553
F_{34}	7534 20141	18967 28166	34100 1452
F_{35}	6937 88244	17537 88339	30832 5486
F_{41}	0 0 14619 4024	0.0 35703 80576	0.0_2 71797 2415
F_{43}	0.0 11685 5913	29068 37526	53676 9185

(p,q)	(6, 3)	(6, 4)	(6, 5)
F_{10}	0.0 11500 46047 4	0.0 27436 07418	0.0 67072 11464 413988
F_{11}	0.0_2 9809 40114 5	24239 36526	60569 09843 27
F_{12}	8815 66302 8	22069 42749	55773 04461 6
F_{13}	8037 98842 2	20366 8457	51924 73834 6
F_{14}	7447 77147 5	19000 2065	48743 90844
F_{15}	6949 83812 8	17851 9853	46039 9523
F_{16}	6542 65850 9	16877 770	43705 440
F_{17}	6185 16985 9	16029 01	41657 40
F_{18}	5881 36480 8	15286 4	39843 2
F_{19}	5607 79351 4	14624	38218
F_{20}	0.0 11564 40995 2	0.0 27012 14376	0.0 64642 84674 0
F_{21}	0.0_2 9632 29044 1	23282 1301	57025 21877 1
F_{22}	8429 47673 8	20711 7684	51415 07564
F_{23}	7527 41740 8	18733 3085	46976 4782
F_{24}	6831 73618 4	17154 781	43348 421
F_{25}	6265 74738 2	15851 45	40305 77
F_{26}	5798 44900 0	14754 6	37708 4
F_{27}	5401 54468	13814	35456
F_{30}	0.0 14562 18106 2	0.0 33963 5096	0.0 80981 00979
F_{31}	12134 17732 2	29175 7059	71094 4144
F_{32}	10553 35095 2	25803 821	63737 579
F_{33}	9374 35649 5	23210 37	57920 09
F_{34}	8458 22393 6	21138 9	53170 0
F_{35}	7717 37598	19434	49193
F_{41}	0.0 17010 60436 7	0.0 40933 96	0.0 99770 14
F_{43}	13164 34035	32578	81226

(p,q)	(5.5, 3.5)				(5,1)				(5,3)			
F_{10}	0.0	30582	12644	25746	0.0_2	72023	00583	92093	0.0	34557	35734	64
F_{11}		26546	86084	76		49301	72645	2311		29305	34984	
F_{12}		23980	61548	53		44687	89140	2958		26250	93614	
F_{13}		21982	57184	13		37613	43764	8036		23865	83829	
F_{14}		20417	40515	3		35273	87818	7399		22065	47190	
F_{15}		19106	28444	1		31313	32791	8846		20548	59534	
F_{16}		18010	93422	2		29863	03990	7079		19313	23280	
F_{17}		17057	22909	7		27202	81435	3412		18229	44513	
F_{18}		16232	53011			26207	13574	9605		17311	57008	
F_{19}		15496	68182			24246	94395	5459		16485	32049	
F_{20}	0.0	29988	43334	47	0.0_2	71268	33847	2171	0.0	33691	4361	
F_{21}		25384	70849	11		50352	37956	5393		27876	9164	
F_{22}		22365	32950	8		42436	28446	8161		24296	2608	
F_{23}		20078	17340	9		36005	60699	8930		21622	8222	
F_{24}		18284	77101	9		32015	37894	0608		19571	5016	
F_{25}		16817	82008	7		28561	37484	7094		17907	8195	
F_{26}		15595	71174			26086	64315	6750		16539	0008	
F_{27}		14554	31596			23867	07199	8967		15379	1272	
F_{30}	0.0	37428	98526	75	0.0_2	86288	73211	0072	0.0	41661	0699	
F_{31}		31632	67070	35		63283	15565	0205		34513	7926	
F_{32}		27708	83437	9		52453	98852	6536		29904	4115	
F_{33}		24743	08599	1		44677	28246	3964		26483	3601	
F_{34}		22409	07979			39269	91764	8601		23836	8820	
F_{35}		20507	64306			35004	29618	8865		21703	7118	
F_{41}	0.0	44139	76962	9	0.0_2	87427	77146	4118	0.0	47859	5043	
F_{43}		34577	05492			62131	43567	6035		36826	5867	

(p,q)	(4.5, 0.5)	(4, 1)	(4, 2)
F_{10}	0.0_2 92262 54376 62253	0.0 22447 15110 78603	0.0 46787 05183 85484
F_{11}	54041 70772 71	15075 47151 53101	36688 13159 3
F_{12}	51903 92766 57	13655 79366 24700	32414 60819 6
F_{13}	40488 58972 61	11391 13901 8343	28702 38520 2
F_{14}	39725 82048 84	10683 54846 9362	26361 58330 0
F_{15}	33379 44055 21	9424 56759 8190	24172 27180 5
F_{16}	33091 94158 60	8992 24034 5928	22635 39837
F_{17}	28820 98492 41	8150 36302 657	21134 16309
F_{18}	28752 90241 36	7857 41531 215	20026 7283
F_{19}	25592 88523 75	7238 98575 211	18911 932
F_{20}	0.0_2 87904 10740 4	0.0 21359 58558 5230	0.0 44631 37590 0
F_{21}	56672 68023 1	14835 89738 2583	34485 27996 6
F_{22}	47781 88986 2	12441 36784 9646	29327 22783 0
F_{23}	39362 74485 8	10483 78993 925	25503 86511 8
F_{24}	35005 34495 7	9291 51139 233	22771 72016
F_{25}	30755 33084 5	8253 73550 307	20563 65465
F_{26}	28121 71649 5	7520 67358 97	18822 3338
F_{27}	25498 41077 8	6859 67811 34	17348 305
F_{30}	0.01 03314 80607 5	0.0 25212 68589 7452	0.0 53666 41186 1
F_{31}	0.0_2 71175 18710 8	18247 57310 959	42020 96677 6
F_{32}	58221 41811 5	15040 49920 634	35475 80772
F_{33}	48739 17655 2	12743 30088 061	30769 96837
F_{34}	42574 92655 4	11161 97323 24	27297 5020
F_{35}	37627 81681 8	9917 14897 78	24555 852
F_{41}	0.0_2 97740 10806 4	0.0 24855 63710 62	0 0 57352 41514
F_{43}	67448 59284 9	17503 16985 68	42278 954

(p,q)	(4, 3)	(3.5, 0.5)	(3.5, 1.5)
F_{10}	0.1 05802 23887 98594	0.0 29425 06376	0.0 56878 34528 16928
F_{11}	0.0 89077 18647 0	16707 12363	41598 43818 34264
F_{12}	79477 82428 6	16142 29434	36830 44713 7939
F_{13}	72000 47811	12379 80701	31799 34336 409
F_{14}	66394 92276	12215 60407	29297 98757 50
F_{15}	61678 6881	10131 51766	26445 65085 52
F_{16}	57857 474	10095 50405	24850 91851 7
F_{17}	54507 38	8682 95670	22933 16886 0
F_{18}	51681 3	8669 71853	21809 83797 8
F_{19}	49127	7509 30751	20401 51372 9
F_{20}	0.0 99181 12915 8	0.0 26772 86258	0.0 53125 02915 1221
F_{21}	81401 10889	16838 16099	38914 35390 323
F_{22}	70598 83493	14141 63570	32701 80774 5
F_{23}	62575 7710	11526 99264	27968 05769 8
F_{24}	56457 871	10209 82786	24805 92808 8
F_{25}	51513 77	8866 22754	22197 76875 3
F_{26}	47458 3	7961 65488	20229 82494
F_{27}	44987	6772 11402	18534 62948
F_{30}	0.1 19928 77647	0.0 30518 51532	0.0 62511 29175 16
F_{31}	0 0 98668 5160	20639 86580	46982 28263 3
F_{32}	85114 759	16759 86479	39067 90944 8
F_{33}	75111 29	13856 75272	33440 31998 1
F_{34}	67404 1	11848 88170	29422 88225 4
F_{35}	63127	9779 34889	26272 03755
F_{41}	0.1 35067 62	0.0 27802 99402	0.0 63550 37680
F_{43}	0.1 05780	18107 21290	45616 59610

(p,q)	(3, 1)	(2.5, 0.5)	(2, 1)
F_{10}	0.0 72361 85511	0.0 98304 08468 705984	0. 24727 84498 60708
F_{11}	47372 29107	53423 09162 00	15591 78369 5977
F_{12}	42908 68512	52153 03957 14	14144 76142 4211
F_{13}	35360 20791	39030 15936 57	11446 39937 5871
F_{14}	33188 43762	38890 55208 25	10768 96044 823
F_{15}	29027 93573	31665 07574 2	9297 94352 69
F_{16}	27728 41064	31863 56442 9	8906 58380 52
F_{17}	24960 99503	27019 92334 4	7934 42883 2
F_{18}	24097 37986	27344 56719 7	7683 17106
F_{19}	22071 73743	23760 70362 4	6974 5399
F_{20}	0.0 65291 41215	0.0 83770 66068 2	0. 20600 48381 0094
F_{21}	44352 11708	50958 56790 0	13511 05496 6456
F_{22}	36976 00200	42643 21047 8	11228 22913 555
F_{23}	30883 86056	34311 09988 6	9262 06211 96
F_{24}	27266 75576	30356 32316 3	8139 68701 50
F_{25}	24089 74568	26269 61439 2	7137 76970 0
F_{26}	21889 31508	23909 43368 7	6464 35674
F_{27}	19888 28666	21426 54391 1	5842 5640
F_{30}	0.0 74546 52912	0.0 91635 27324 9	0. 22411 98260 570
F_{31}	53060 17075	60560 82885 1	15640 83450 02
F_{32}	43444 84144	48903 00992 9	12679 86033 20
F_{33}	36572 58458	40271 94375 3	10587 41463 9
F_{34}	31902 54122	34844 53199 7	9189 28942
F_{35}	28234 29907	30490 87297 5	8092 7849
F_{41}	0.0 71026 59138	0.0 80180 45104 5	0. 20403 20662 6
F_{43}	49483 35392	54000 40399 4	14054 4647

Table 9. Natural logarithm

n	$\log_e n$						
2	0.69314	71805	59945	30941	72321	21458	17657
3	1.09861	22886	68109	69139	52452	36922	52570
4	1.38629	43611	19890	61883	44642	42916	35314
5	1.60943	79124	34100	37460	07593	33226	18764
6	1.79175	94692	28055	00081	24773	58380	70227
7	1.94591	01490	55313	30510	53527	43443	17973
8	2.07944	15416	79835	9282	16963	64374	52970
9	2.19722	45773	36219	38279	04904	73845	05141
10	2.30258	50929	94045	68401	79914	54684	36421
11	2.39789	52727	98370	54406	19435	77965	12930
12	2.48490	66497	88000	31022	97094	79838	87884
13	2.56494	93574	61536	73605	34874	41565	31860
14	2.63905	73296	15258	61452	25848	64901	35630
15	2.70805	02011	02210	06599	60045	70148	71334
16	2.77258	87222	39781	23766	89284	85832	70627
17	2.83321	33440	56216	08024	95346	17873	12654
18	2.89037	17578	96164	69220	77225	95303	22798
19	2.94443	89791	66440	46000	90274	31887	85353
20	2.99573	22735	53990	99343	52235	76142	54078

References

1) T. Murai, Prog. Theor. Phys. **7** (1952), 345.
2) M. Kotani, A. Amemiya and T. Simose, Proc. Phys. Math. Soc. Japan **20** (1938), Extra number 1.
3) R. S. Mulliken, C. A. Rieke, D. Orloff and H. Orloff, J. Chem. Phys. **17** (1949), 1248.
4) G. Araki and W. Watari, Prog. Theor. Phys. **6** (1951), 961.
5) H. J. Kopineck, Z. Naturforschung, **5** (1950), 490; **6** (1951), 177.
6) A. L. Sklar, J. Chem. Phys. **7** (1939), 984.
7) M. G. Mayer and K. J. McCallum, Rev. Mod. Phys. **14** (1942), 248.
8) J. F. Mulligan, J. Chem Phys. **19** (1951), 347.
9) M. P. Barnett and C. A. Coulson, Phil. Trans. Roy. Soc London **A243** (1951), 221.
10) C. C. J. Roothaan, J. Chem. Phys. **19** (1951), 1445.
11) K. Rudenberg, J. Chem. Phys. **19** (1951), 1459.
12) R. G. Parr and B. L. Crawford, J. Chem. Phys. **16** (1948), 1049.

Errata

T. Murai, **Electronic States of Ethylene Molecule**

(Vol. 7, No. 4, pp. 345—352)

Eq. (15) *for* $\sum_{k=1}^{n-1}$ *read* $\sum_{k=0}^{n-1}$

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Molecular Structure and Absorption Spectra of Carotenoids*

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An assemblage of π-electrons in the chain of carotenoid molecules is discussed, according to Tomonaga's method, on the basis of an assumption that the electrons are kept in a pipe whose length is equal to the chain length of conjugated double bonds. The spin degrees of freedom of electrons are taken into account though Tomonaga disregarded them. The one-dimensional potential of two-electron forces is assumed to be given by an average of the Coulomb repulsive potential over a section of the pipe. The calculated values of absorption maxima are in good agreement with experiment for carotenoids. The adequacy of the method is discussed.

Introduction

The relation between absorption spectra and molecular structures of a certain kind of organic dyes have long been known.[1)2)] Kuhn[3)4)] first tried to account for the relation in terms of quantum mechanics by assuming a model in which π-electrons are kept in a one-dimensional domain restricted by high potential barriers at both ends. His idea provided us with an interesting way for theory on the absorption spectra, but unfortunately his theoretical result was not in good agreement with experiment for carotenoids. He neglected interactions between electrons. This point was a defect of his theory because the interaction energy is expected to be more important compared with the kinetic energy in case of long molecules.

Carotenoid molecules have long chains of conjugated double bonds. When we plot observed wave lengths of their absorption maxima as a function of the number of the conjugated double bonds we obtain a monotone increasing and downwards concave curve. If we assume the π-electrons to be free we can not account for the concavity but we have a straight line. The reason for the concavity may be attributed to two causes: The effect of the periodic field due to the molecular core; and the interaction between π-electrons. The first was considered by Kuhn to a certain extent. In the present paper the second effect will be fully discussed, according to Tomonaga's method, on the basis of an assumption that an assemblage of π-electrons in the chain of carotenoid molecules can be considered as being kept in a pipe whose length is equal to the chain length of conjugated double bonds.

The theoretical values of absorption maxima will be found to be in good agreement with experiment for carotenoids as will be shown in Table 1 and Fig 2. We shall further

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find that the energy due to the Coulomb repulsion between π-electrons is very large in accordance with our first expectation. The agreement of the present theory with experiment does not mean that the concavity of the above mentioned curve for absorption maxima is solely due to the Coulomb interaction. If the other effect has the similar tendency the present result effectively involves it because the value of a parameter is adjusted to fit theory and experiment.

§ 1. Eigenvalue Problem of One-dimensional N-electron System

We shall consider a one-dimentional longitudinal motion of electrons enclosed in a pipe according to Tomonaga's method. We shall discuss the eigenvalue problem of energy of the system taking into account the spin of the electron whereas Tomonaga disregarded it. The one-electron wave function has therefore two components in the present theory. This is an only point which discriminates the present theory from Tomonaga's. The whole reasoning is thus quite similar to the latter. The same reasoning will not be repeated here in detail but merely a short account of different points will be given introducing new operators which are more familiar in the quantization in field theory.

If we neglect the interaction between electrons the eigenvalues of one-electron energy are given by

$$\varepsilon(n)=\left(\frac{h}{L}\right)^2\frac{n^2}{2m}, \qquad n=0,\ \pm 1,\ \pm 2,\cdots \tag{1·1}$$

and the corresponding one-electron eigenfunctions are

$$\frac{1}{\sqrt{L}}\exp\left(\frac{2\pi i}{L}nx\right) \tag{1·2}$$

where m is the electron mass, and L is the length of the pipe. The ground state of the total system is such that in which one-electron levels are compactly occupied by electrons in energy order from the lowest according to the Pauli principle. We assume that all levels up to $\varepsilon(n_0)$ are just completely occupied in this ground state where n_0 is a positive integer. We shall refer to $\varepsilon(n_0)$ (the highest occupied level) or n_0 as the Fermi maximum.

Let $\psi_1(x)$ and $\psi_2(x)$ be two components of the quantized wave function describing the state of the total system. These are expanded in a series of eigenfunctions given by (1·2) as follows:

$$\psi_\lambda(x)=\sum_{n=-\infty}^{\infty}\psi_{\lambda n}\frac{1}{\sqrt{L}}\exp\left(\frac{2\pi i}{L}nx\right), \qquad (\lambda=1,\ 2) \tag{1·3}$$

in $-L/2\leqq x\leqq L/2$. The coefficient operators satisfy the Fermion anti-commutation relation:

$$\begin{aligned}&\{\psi_{\lambda n}\psi^*_{\lambda' n'}\}=\delta_{\lambda\lambda'}\delta_{nn'},\\ &\{\psi_{\lambda n}\psi_{\lambda' n'}\}=\{\psi^*_{\lambda n}\psi^*_{\lambda' n'}\}=0\end{aligned} \tag{1·4}$$

where the asterisk indicates a Hermitian conjugate and the brace denotes an anti-commutator.

We introduce new operators by

$$a_\nu = \frac{1}{\sqrt{2\nu}} \sum_{n>0} \sum_{\lambda=1}^{2} \psi^*_{\lambda\, n-\nu/2}\, \psi_{\lambda\, n+\nu/2}\,,$$
$$a_{-\nu} = \frac{1}{\sqrt{2\nu}} \sum_{n<0} \sum_{\lambda=1}^{2} \psi^*_{\lambda\, n+\nu/2}\, \psi_{\lambda\, n-\nu/2} \qquad (1\cdot5)$$

where ν is a positive integer. These correspond to Tomonaga's density operators except a factor. By virtue of the anti-commutation relation for $\psi_{\lambda n}$ they satisfy the Boson commutation relation (the bracket denotes a commutator) :

$$[a_\mu\, a^*_\nu] = \delta_{\mu\nu}\,; \qquad [a_\mu\, a_\nu] = [a^*_\mu a^*_\nu = 0 \qquad (1\cdot6)$$

under the following restriction :

$$\left.\begin{array}{l} \text{In the region } |n| < 3n_0/4, \text{ there is no hole ;} \\ \text{In the region } |n| > 5n_0/4, \text{ there is no electron ;} \\ |\nu| < n_0/2. \end{array}\right\} \qquad (1\cdot7)$$

Thus we can replace a Fermion system, described by $\psi_{\lambda n}$, by a Boson system described by a_ν.

From (1·1) and (1·5) we have the relation $da_\nu/dt = -(i/\hbar)(h/L)^2(n_0/m)|\nu|a_\nu$ under the above mentioned restriction. By virtue of $da_\nu/dt = (i/\hbar)[\mathfrak{H} a_\nu]$ and the commutation relation for a_ν this means that, when the interaction between electrons is neglected, the energy of the total system is given by

$$\mathfrak{H} = \sum_\nu T_\nu\, a^*_\nu\, a_\nu + \mathfrak{H}_0 \qquad (1\cdot8)$$

where $\mathfrak{H}_0$ denotes a term independent of a_ν, and T_ν is defined by

$$T_\nu = \left(\frac{h}{L}\right)^2 \frac{n_0}{m}|\nu|\,. \qquad (1\cdot9)$$

Since $a^*_\nu a_\nu$ represents the number of Bosons, $\mathfrak{H}_0$ stands for the energy of the ground state in which all of the one-electron levels up to the Fermi maximum are completely occupied.

The interaction energy due to two-electron forces is represented in terms of a density operator, $\rho(x)$, and one-dimensional potential, $J(x-x')$, of the two-electron force as follows :

$$H_{int} = \frac{1}{2}\iint \rho(x)\rho(x')J(x-x')\,dx\,dx' - \frac{1}{2}\int \rho(x)J(0)\,dx. \qquad (1\cdot10)$$

The density operator is represented in terms of a_ν :

$$\rho(x) = \sum_{\lambda=1}^{2} \psi^*_\lambda(x)\psi_\lambda(x)$$
$$= \sum_{\nu\neq0} \frac{\sqrt{2|\nu|}}{L}\left\{a_\nu \exp\left(\frac{2\pi i}{L}\nu x\right) + a^*_\nu \exp\left(-\frac{2\pi i}{L}\nu x\right)\right\} + \frac{N}{L} \qquad (1\cdot11)$$

where N is the total number of electrons in the system. It follows from these two equations that

$$H_{int}=\sum_{\nu\neq 0}|\nu|J_\nu(2a_\nu^*a_\nu+a_\nu^*a_{-\nu}^*+a_\nu a_{-\nu}+1)+\frac{1}{2}N^2J_0-\frac{1}{2}NJ(0) \tag{1·12}$$

where J_ν is the Fourier coefficient of the potential function $J(x)$:

$$J_\nu=J_{-\nu}=\frac{1}{L}\int_{-L/2}^{+L/2}J(x)\exp\left(\frac{2\pi i}{L}\nu x\right)dx\,. \tag{1·13}$$

Adding $\mathfrak{H}$ and H_{int} we have the total Hamiltonian of the system as follows :

$$H=\sum_\nu(T_\nu+U_\nu)a_\nu^*a_\nu+(1/2)\sum_\nu U_\nu(a_\nu^*a_{-\nu}^*+a_\nu a_{-\nu}+1)+W \tag{1·14}$$

where

$$\begin{aligned}&U_\nu=2|\nu|J_\nu\,,\\&W=(N^2/2)J_0-(N/2)J(0)+\mathfrak{H}_0\,.\end{aligned} \tag{1·15}$$

We see that this total Hamiltonian has the same form as Tomonaga's result. Only a difference is the factor 2 in the definition of U_ν. In Tomonaga's result this factor was lacking. The reason for its appearing is that we are assuming two degrees for the spin freedom. The diagonalization of H can immediately be carried out by an unitary transformation as follows :

$$b_\nu=\frac{1}{2}\left(\sqrt[4]{1+\delta_\nu}+\frac{1}{\sqrt[4]{1+\delta_\nu}}\right)a_\nu+\frac{1}{2}\left(\sqrt[4]{1+\delta_\nu}-\frac{1}{\sqrt[4]{1+\delta_\nu}}\right)a_{-\nu}^* \tag{1·16}$$

where

$$\delta_\nu=\frac{2U_\nu}{T_\nu}=\left(\frac{L}{h}\right)^2\frac{4m}{n_0}J_\nu\,. \tag{1·17}$$

The transformed form of the Hamiltonian is

$$H=\sum_\nu b_\nu^*b_\nu T_\nu\sqrt{1+\delta_\nu}+E_0 \tag{1·18}$$

where

$$E_0=\sum_\nu\frac{T_\nu}{2}(\sqrt{1+\delta_\nu}-1)+W\,. \tag{1·19}$$

The operator $b_\nu^*b_\nu$ represents the number of Bosons whose energy is equal to $T_\nu(1+\delta_\nu)^{1/2}$ and its eigenvalues are given by $N_\nu=0,\ 1,\ 2,\ 3,\ldots$. The energy eigenvalue of the total system is therefore equal to

$$E=\sum_\nu N_\nu T_\nu\sqrt{1+\delta_\nu}+E_0\,. \tag{1·20}$$

§ 2. Fourier Coefficient of Interaction Potential and Applicability Condition

As is well known, the Coulomb repulsive potential is expanded in the Fourier series in a parallelepiped with the edge length L_1, L_2 and L_3 as follows:

$$\frac{e^2}{r}=\frac{4\pi e^2}{L_1L_2L_3}\left\{\frac{1}{k_0^2}+\sum_{k\neq 0}\frac{1}{\mathbf{k}^2}\exp(i\mathbf{kx})\right\} \tag{2·1}$$

where $r=|\mathbf{x}|$ and the approximate value of $\mathbf{k}^2$ is given by

$$k_j=(2\pi/L_j)n_j\,, \quad (j=1,\,2,\,3\,;\ n_j=0,\ \pm1,\ \pm2,\ldots\,;\ \mathbf{k}\neq 0)\,. \tag{2·2}$$

We assume that $J(x)$ in the preceding section is given by an average of the Coulomb potential of two-electron forces over the transverse section of the pipe in which electrons are enclosed. If the section is rectangular and its area is A we have $L_2L_3=A$ and $L_1=L$. The Fourier coefficient of $J(x)$ is then given by

$$J_\nu=\frac{e^2L}{\pi A}\,\frac{1}{\nu^2}\,, \quad (\nu=\pm1,\ \pm2,\ \ldots) \tag{2·3}$$

and substituting this for J_ν in (1·17) we have

$$\delta_\nu=\frac{\delta}{\nu^2}, \quad \delta=\left(\frac{L}{\pi}\right)^3\frac{1}{aAn_0} \tag{2·4}$$

where a is the Bohr radius ($a=\hbar^2/(me^2)$).

Now we shall derive a necessary condition which must be satisfied under the restriction given by the first two of (1·7). As was discussed by Tomonaga, this can be expressed in the form that the expectation value of $\mathfrak{H}-\mathfrak{H}_0$ should be less than the possible maximum kinetic excitation energy for the state in question. The former is obtained from (1·8) and (1·16) as follows:

$$\langle\mathfrak{H}-\mathfrak{H}_0\rangle=\left(\frac{h}{L}\right)^2\frac{n_0}{2m}\left\{\sum_\nu|\nu|(c_\nu+2)N_\nu+\sum_{\nu=1}^{\infty}\nu c_\nu\right\} \tag{2·5}$$

and the latter is

$$\left(\frac{h}{L}\right)^2\frac{n_0^2(n_0+4)}{4m} \tag{2·6}$$

where

$$c_\nu=\sqrt{1+\delta_\nu}+\frac{1}{\sqrt{1+\delta_\nu}}-2\,. \tag{2·7}$$

The necessary condition is then

$$\frac{2}{n_0(n_0+4)}\left\{\sum_\nu|\nu|(c_\nu+2)N_\nu+\sum_{\nu=1}^{\infty}\nu c_\nu\right\}<1\,. \tag{2·8}$$

From (2·7) we have $\delta_\nu^2=(4c_\nu+c_\nu^2)(1+\delta_\nu)$, therefore $(\delta_\nu^2/4)>c_\nu$, and consequently

$$\sum_{\nu=1}^{\infty}\nu c_\nu<\sum_{\nu=1}^{\infty}\frac{\nu}{4}\delta_\nu^2=\frac{\delta^2}{4}\sum_{\nu=1}^{\infty}\frac{1}{\nu^3}\,. \tag{2·9}$$

The value of $\sum' \nu^{-3}$ is 1.2020*. Therefore the necessary condition is satisfied when

$$\Delta < 1 \tag{2·10}$$

where

$$\Delta = \frac{2}{n_0(n_0+4)} \{\sum_{\nu}' |\nu| (c_\nu + 2) N_\nu + 0.3005\, \delta^2\}. \tag{2·11}$$

Fig. 1 Chemical Structure of Carotenoids I.

(1) Dibenzyl-butadiene

(2) Hepaxanthin

(3) Dibenzyl-hexatriene

(4) Iso-desmethyl-axerophtene

(5) Iso-axerophtene

(6) Axerophtene

(7) Desmethyl-axerophtene

(8) Iso-anhydro-vitamin A

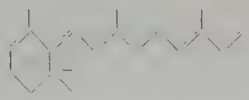
(9) 15 Ethyl-axerophtene

(10) Dihydro-crocetin

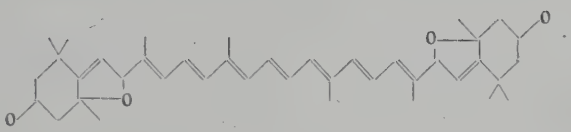
H and C are not written. CC and CO single and double bonds only are indicated but not CH bonds. At corners and ends of bond segments there are carbons. H's should be so added that valences of carbons are four and those of oxygens are two. Therefore side branches, for example, mean methyl radicals.

* $\zeta(z) = \sum_{n=1}^{\infty} \frac{1}{n^z}$ is known as Rieman's zeta function. Its values at $z=2n+1$ $(n=0, 1, 2, \cdots)$ have not yet known in general. We obtain $\zeta(3)=1.2020$ by the numerical calculation.

(11) Anhydro-vitamin A

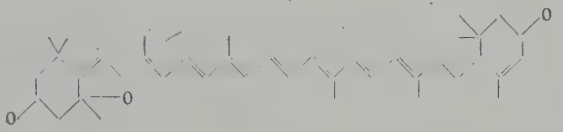


(12) Auroxanthin ?

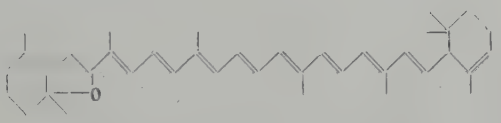


(13) Dihydro-β-carotene

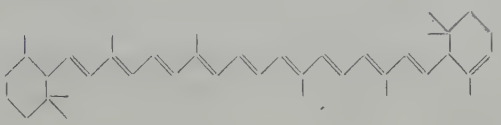
(14) Chrysanthemaxanthin
(Flavoxanthin)



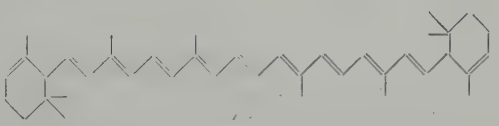
(15) Flavochrom



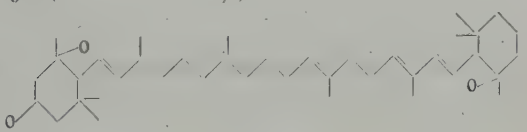
(16) 5, 6-Dihydro-α-carotene



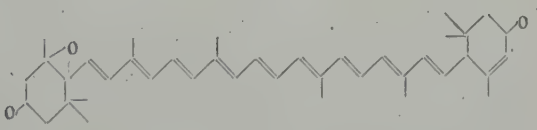
(17) ε_1-carotene



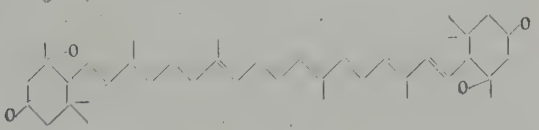
(18) Cryptoxanthin-di-epoxyde



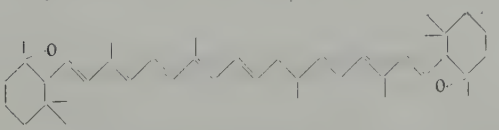
(19) Iso-antheraxanthin



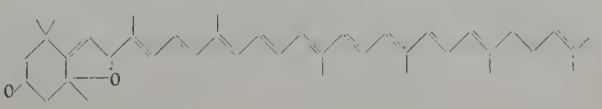
(20) Violaxanthin



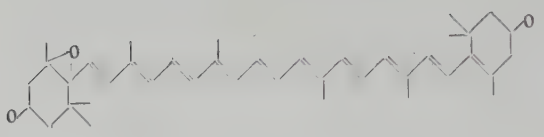
(21) β-carotene-di-epoxyde



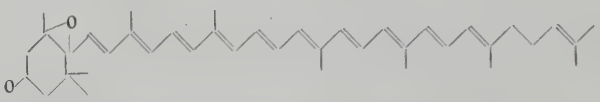
(22) Rubichrom



(23) Antheraxanthin



(24) Rubixanthin
-mono epoxyde



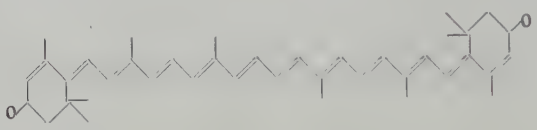
(25) Astaxanthin

(26) Lycoxanthin

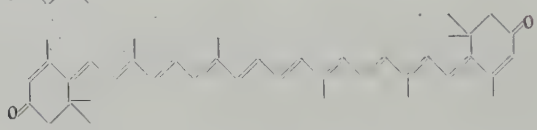
(27) Lycophyll

(28) Lycopene

(29) Eschscholtzxanthin

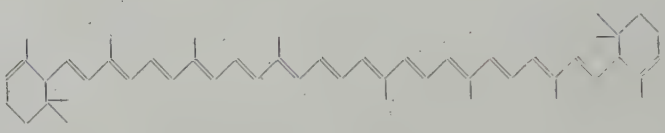


(30) Rhodoxanthin

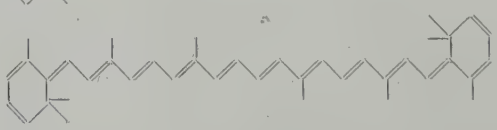


(31) Rhodoviolascin

(32) Decapreno-ε-carotene

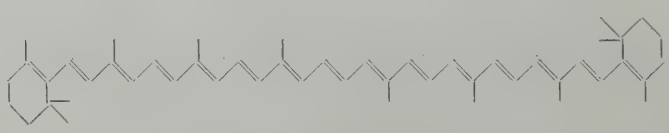


(33) Anhydro-
eschscholtzxanthin

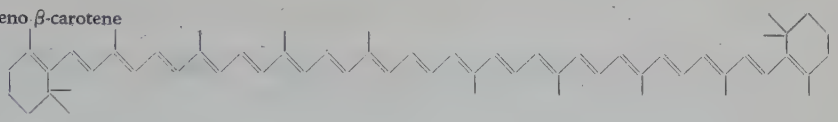


(34) Dehydro-lycopene

(35) Decapreno-β-carotene



(36) Dodecapreno-β-carotene



§ 3. Absorption Spectra of Carotenoids

We shall apply the result of the preceding sections to the absorption spectra of carotenoids. Carotenoid molecules consist of a long chain of carbon atoms, methyl branches, and ring or non-ring shaped ends, as is shown in Fig. 1. The chain of carbon atoms is connected by a series of conjugated double bonds. The single bond and one of the double bonds in the chain are linked by so-called σ-electrons in the sp^2 states. The remainder of the double bonds is linked by π-electrons. We assume that the assemblage of π-electrons in the chain of conjugated double bonds of a carotenoid molecule forms the system of electrons discussed in the preceding sections and the remainder of the molecule plays a rôle of the pipe. If we put $N_1=1$ and $N_\nu=0$ for $\nu\neq 1$ in (1·20) we have the first excitation energy of the molecule. Since we have assumed that one-electron levels up to the Fermi maximum, n_0, can be just completely occupied by N electrons without interactions we have $N=2(2n_0+1)$. Double bonds contain two π-electrons. Therefore N is equal to $2j$ if j is the number of conjugated double bonds. The first excitation energy is then given by

$$\Delta E=2\left(\frac{\pi}{L}\right)^2(j-1)\sqrt{1+\delta}\,,$$
$$\delta=\left(\frac{L}{\pi}\right)^3\frac{2}{A(j-1)} \qquad (3\cdot1)$$

where all quantities are measured in atomic units.

We assume that the effective length of the chain of the carotenoid corresponding to the pipe is simply given by

$$L=j(l_1+l_2)=(N/2)(l_1+l_2) \qquad (3\cdot2)$$

where l_1 and l_2 are the lengths of the single and double bonds respectively. These lengths have not yet measured for carotenoids. Therefore we assume a fixed value, $l_1+l_2=2.8\text{Å}=5.2915$ atomic units, which is adopted from experimental values for smaller molecules.[6] Then we have only a value of A, the sectional area of the pipe, as a parameter which can adjust in order that Eq. (3·1) agrees with experiment. We fix the value of A by comparing (3·1) with the observed value of absorption maximum of decapreno-β-carotene, and we obtain $A=724.288$ atomic units ($A^{1/2}=26.9126$ atomic units). The wave length at the maxima of absorption spectra of carotenoids is assumed to be given by $\lambda=hc/(\Delta E)$. Then we have the following equation for the wave length of absorption maxima:

$$\lambda=\frac{j}{0.015472\left(1-\frac{1}{j}\right)\sqrt{1+\frac{0.013195j^2}{1-\frac{1}{j}}}} \qquad (3\cdot3)$$

where λ is measured in $m\mu$.

The calculated values are compared with experiment[1)7)–57)] in Table 1 and Fig. 2 where two dibenzylpolyenes are included for the sake of comparison convenience. The absorption spectra of carotenoids have usually three maxima of which the central ones are strongest. In the fourth column of Table 1 the observed wave lengths of the strongest maxima are shown. The fluctuation of observed wave lengths of absorption maxima for the definite number of conjugated double bonds may be due to end structures of molecules or partial admixtures of cis-structures. The positions of absorption maxima depend on solvent too. The influence of solvents is known from the observations in which the same carotenoid is dissolved in various solvents. The experimental data in Table 1 are so chosen that the influence of solvents are as similar as possible. The influence may be corrected to a standard solvent, but we give here only original data without the correction because we can not discuss the minute fluctuation in the present theory. We see that the theoretical values are in good agreement with experiment.

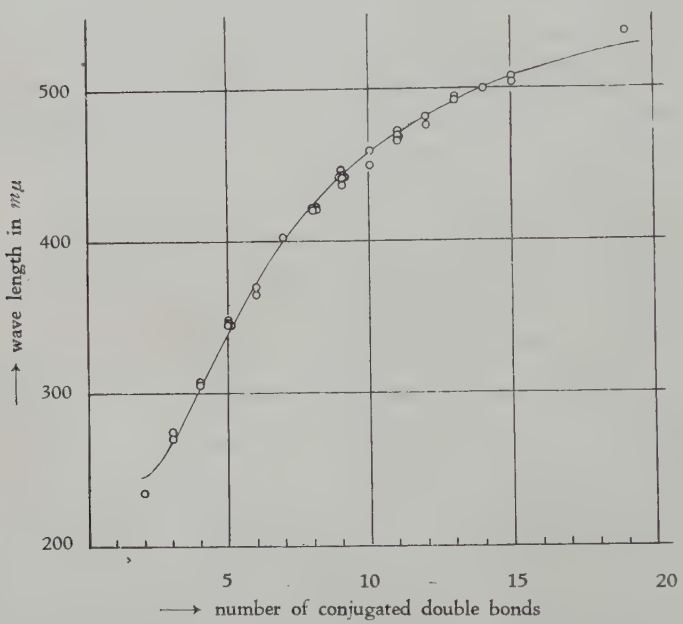


Fig. 2. Relation between Absorption Maxima and Number of Conjugated Double Bonds of Carotenoids.
Full curve: theoretical relation
Circles: observed wave lengths of absorption maxima

As is seen from Eq. (1·17), Eq. (1·20) and Eq. (2·4), δ is an indicator of the strength of interaction between electrons. When there is no interaction δ vanishes. It was pointed out by Tomonaga that if we expand the right-hand side of Eq. (1·20) in power series in δ, the terms up to quadratic in δ are the same as the usual Thomas-Fermi approximation including the exchange effect plus the second order perturbation term of Euler when the spin is neglected. In short δ is a ratio of the Coulomb interaction

Table 1. Absorption Maxima of Carotenoids I

j: number of conjugated double bonds
N: number of π-electrons
$\lambda_{calc.}$, $\lambda_{obs.}$: wave lengths of calculated and observed absorption maxima measured in $m\mu$
solv: solvent; H: hexane; A: ethylalcohol; B: *Benzin*; P: petroleum ether; C: cyclohexane

j	N	$\lambda_{calc.}$	$\lambda_{obs.}$	solv.	str.	carotenoids
2	4	246	235	H	(1)	Dibenzyl-butadiene[1]
3	6	268	275	A	(2)	Hepaxanthin[24][31]
			270	H	(3)	Dibenzyl-hexatriene[1]
4	8	305	306	A	(4)	Iso-desmethyl-axerophtene[40]
			308	A	(5)	Iso-axerophtene[39]
5	10	340	346	A	(6)	Axerophtene[35][38]
			346	A	(7)	Desmethyl-axerophtene[36]
			347	A	(8)	Iso-anhydro-vitamine A[33][50]
			348	A	(9)	15 Ethyl-axerophtene[41]
6	12	371	365	H	(10)	Dihydro-crocetin[1][8][15]
			370	A	(11)	Anhydro-vitamin A[33][50]
7	14	399	403	A	(12)	Auroxanthin[21]
8	16	422	421	H	(13)	Dihydro-β-carotene[17]
			422	H	(14)	Chrysanthemaxanthin[19][21] (Flavoxanthin[7][19][21])
			422	P	(15)	Flavochrom[23]
9	18	441	438	H	(16)	5, 6-Dihydro-α-carotene[51][52]
			439	P	(17)	ε_1-carotene[42][43]
			442	A	(18)	Cryptoxanthin-di-epoxyde[27][32]
			442	B	(19)	Iso-antheraxanthin[21][26][34]
			442	A	(20)	Violaxanthin[1][18][21]
			443	P	(21)	β-carotene-di-epoxyde[22]
			447	P	(22)	Rubichrom[29]
10	20	457	450	A	(23)	Antheraxanthin[21][37]
			461	P	(24)	Rubixanthin-mono-epoxyde[29]
11	22	471	466	H	(25)	Astaxanthin[18]
			471	A	(?)	Rhodopin[18]
			472	B	(26)	Lycoxanthin[57]
			473	B	(27)	Lycophyll[57]
			473	H	(28)	Lycopene[1][17][47][54]
12	24	483	478	C	(29)	Eschscholtzxanthin[45]
			482	H	(30)	Rhodoxanthin[10][18]
13	26	493	493	H	(31)	Rhodoviolascin[18]
			495	P	(32)	Decapreno-ε-carotene[46]
14	28	501	500	P	(33)	Anhydro-eschscholtzxanthin[45]
15	30	508	504	H	(34)	Dehydro-lycopene[25][47]
			508	C	(35)	Decapreno-β-carotene[44]
19	38	528	537	C	(36)	Dodecapreno-β-carotene[47]

energy to the kinetic energy. The numerical values of δ are shown in Table 2. We see that δ is large for long molecules, that is, the case of long molecules is of so-called strong coupling. To the cases of these long molecules the perturbation theory can not be applied. In this respect these cases of strong coupling are especially interesting from the theoretical point of view.

§ 4 Discussion on Various Approximations

The present scheme for electronic levels of carotenoid molecules has been derived assuming a quite simplified model. Therefore the present theory contains various assumptions. The adequacy of these will be examined in what follows.

The theoretical absorption maxima shown in Table 1 are calculated by Eq. (3·1) or (3·3). Strictly speaking, Eq. (3·1) can not be applied to the case of even j because the number, j, of conjugated double bonds should satisfy an equation $j=2n_0+1$ for $n_0=0, 1, 2, \cdots$ (the Fermi maxima). Nevertheless we have assumed the equation to hold for even j too. This may be justified if the same law holds for even j as well as odd. An adequacy of the last assumption is quite possible when the equation is derived in an exact way.

We have assumed that π-electrons are enclosed in a straight pipe whereas carotenoid molecules are of zigzag shape. The shape may shorten the effective length of the pipe, as is seen from the observed shift of absorption maxima due to the cis-trans isomerism.[37) 81)] The length adopted for l_1+l_2 in the preceding section is in fact the shortest of observed values. The shape influence may be included in the effective sectional area, A, of the pipe to a certain extent.

The square root of A means an effective lateral extension of the pipe. It amounts to about five times the value of l_1+l_2. This can be considered as being reasonable because it indicates a long range property of the Coulomb interaction.

As has been mentioned in (1·7), our final equation (1·20) can be applied to the case in which N_ν do not vanish only for $|\nu|<n_0/2$. In the present case of carotenoids this is equivalent to the condition that j is larger than 5. We see from Table 1 that our theoretical values are in agreement with experiment even for $j\leqq 5$. The values of Δ defined by (2·11) are shown in Table 2. We find that the applicability condition, (2·10), is satisfied for all cases except for $j=2$.

In Table 1 we have shown observed absorption maxima which nearly agree with theoretical values. There are many

Table 2. Strength of Couplings and Applicability Indicators
$\delta<1$: weak coupling
$\delta>1$: strong coupling
$\Delta<1$: applicable case

j	δ	Δ
2	0.1056	1.783
3	0.1781	0.807
4	0.2815	0 494
5	0.4123	0.347
6	0.5700	0.265
7	0.7543	0.214
8	0.9651	0.183
9	1.2024	0.162
10	1.4661	0.149
11	1.7562	0.142
12	2.0728	0.138
13	2.4158	0.138
14	2.7851	0.140
15	3.1810	0.145
16	3.6031	0.151
17	4.0517	0.159
18	4.5268	0.168
19	5.0280	0.179
20	5.5558	0.191

carotenoids whose absorption maxima do not agree with theory. They are shown in Table 3. The disagreement may be partly due to end structures of their molecules or their cis-admixture, but not wholly. The real reason may only be disclosed by an exact theory in an orthodox way. We may obtain a better agreement of theory with experiment by introducing a certain modification according to circumstances. For example, we may adopt different values of L corresponding to different kinds of end structures. However, this is meaningless because the present theory does not contain such a complex nature. Its distinction is in its simplicity.

There is another case in which the chain of conjugated double bonds had an end or both of CO double bonds. The examples are azafrin, crocetin, bixin, fucoxanthin, capsorubin, citraurin, capsanthin, myxoxanthin, torularhodin, their derivatives and derivatives of other carotenoids in allied structures. If we replace the CO double bonds by an effective CC bond we can account for their absorption maxima as has generally been well known. However the correction is without a scope of the present theory as is discussed above.

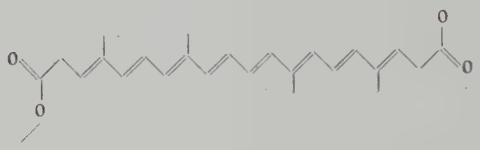
Table 3. Absorption Maxima of Carotenoids II

j	N	λ_{calc}	λ_{obs}	solv.	str.	Carotenoids
4	8	305	295	H	(37)	1,8-Dimethyl-octatetraene[9]
8	16	422	400	A	(38)	Dihydro-bixin[18]
			402	H	(39)	Dihydro-methyl-bixin[1] [18]
9	18	441	427	A	(40)	Mutatoxanthin[21]
			423	A	(41)	Citroxanthin[20] [22] [30]
			430	A	(42)	Cryptoflavin[27] [52]
10	20	457	446	H	(43)	α-Carotene[1] [17] [51] [55]
			445	H	(44)	5, 6-Dihydro-β-carotene[47] [51] [52]
			446	H	(45)	Lutein (Xanthophyll)[1] [18] [55]
			447	P	(46)	β-Carotene-mono-epoxyde[22]
			449	A	(47)	Cryptoxanthin-mono-epoxyde[27] [52]
11	22	471	449	H	(48)	Dihydro-rhodoxanthin[10]
			451	H	(49)	Cryptoxanthin[11] [13] [20]
			452	H	(50)	β-Carotene[17] [49] [51] [55]
			454	A	(51)	Zeaxanthin[1] [15] [23]
			460	H	(52)	Gazaniaxanthin[53]
			462	H	(53)	γ-Carotene[47] [54] [56]
			462	H	(54)	Rubixanthin[12] [14]
12	24	483	473	H	(55)	Dehydro-β-carotene[16] [17] [47]
15	30	508	471	C	(56)	1,18-Diphenyl-3, 7, 12, 16-tetramethyl-octadeca-nonaene[48]

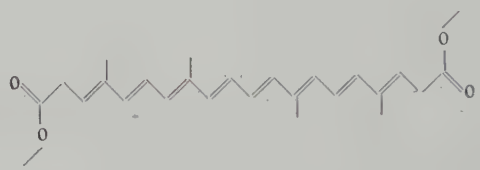
Fig. 3. Chemical Structures of Carotenoids II

(37) 1, 8-Dimethyl-octatetraene

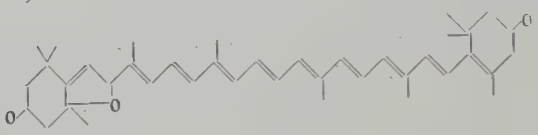
(38) Dihydro-bixin



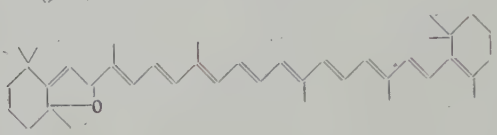
(39) Dihydro-methyl-bixin



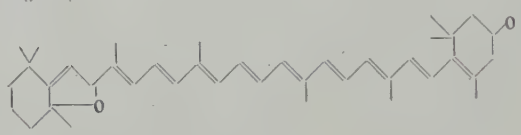
(40) Mutatoxanthin



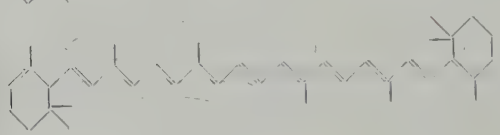
(41) Citroxanthin



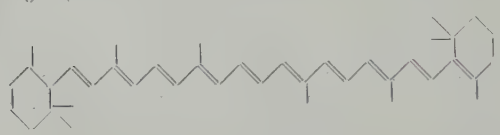
(42) Cryptoflavin



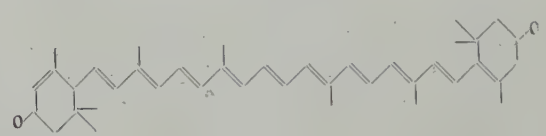
(43) α-Carotene



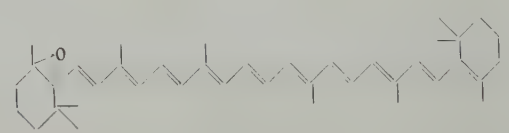
(44) 5, 6 Dihydro-β-carotene



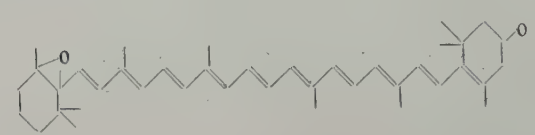
(45) Lutein (Xanthophyll)



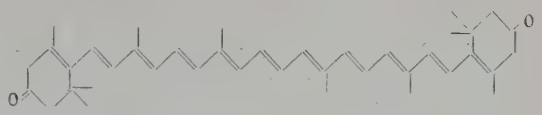
(46) β-Carotene-mono-epoxyde



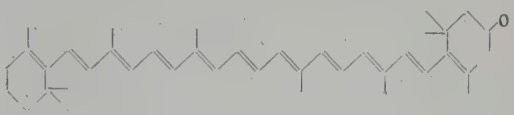
(47) Cryptoxanthin-mono-epoxyde



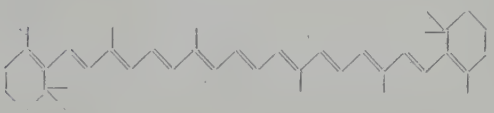
(48) Dihydro-rhodoxanthin



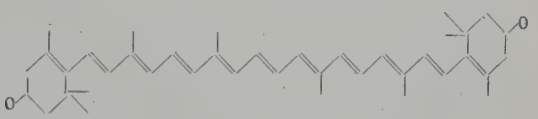
(49) Cryptoxanthin



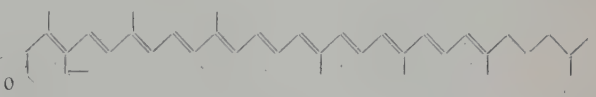
(50) β-Carotene



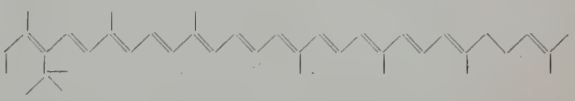
(51) Zeaxanthin



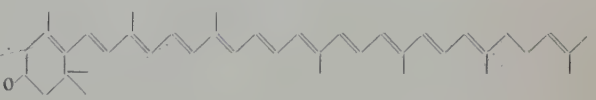
(52) Gazaniaxanthin ?



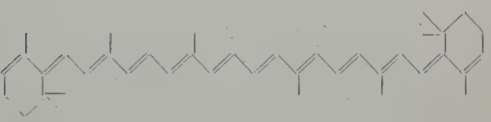
(53) γ-Carotene



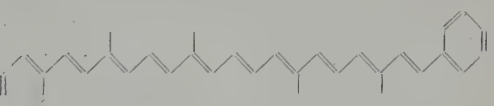
(54) Rubixanthin



(55) Dehydro-β-carotene



(56) 1, 18-Diphenyl-3, 7, 12, 16-tetramethyl-octadeca-nonaene



References

1) A. Smakula, Z. ang. Chem. **47** (1934), 657.
2) K. W. Hausser, R. Kuhn and coworkers, Z. phys. Chem. (B) **29** (1935), 363, 371, 378, 384, 391, 417.
3) H. Kuhn, Helv. Chim. Acta **31** (1948), 1441; **32** (1949), 2247; **34** (1951), 1308, 2371.
4) H. Kuhn, J. Chem. Phys. **17** (1949), 1198.
5) S. Tomonaga, Prog. Theor. Phys. **5** (1950), 544.
6) Landolt-Börnstein, *Zahlenwerte und Funktionen* Bd. 1, Tl. 2 (1951).
7) R. Kuhn und H. Brockmann, Z. physiol. Chem. **213** (1932), 192.
8) A. Smakula, Z. ang. Chem. **48** (1935), 152.
9) R Kuhn, Z. ang. Chem. **50** (1937), 703.
10) R. Kuhn und H. Brockmann, Ber. deutsch. chem. Ges. **66** (1933), 828.

11) R. Kuhn und C. Grundmann, Ber. deutsch. chem. Ges. **66** (1933), 1746.
12) R. Kuhn und C. Grundmann, Ber. deutsch. chem. Ges. **67** (1934), 339.
13) R. Kuhn und C. Grundmann, Ber. deutsch. chem. Ges. **67** (1934), 593.
14) R. Kuhn und C. Grundmann, Ber. deutsch. chem. Ges. **67** (1934), 1133.
15) H. v. Euler, P. Karrer, E. Klussmann und R. Morf, Helv. Chim. Acta 15 (1932), 502.
16) P. Karrer und G. Schwab, Helv. Chim. Acta **23** (1940), 578.
17) P. Karrer und A. Rüegger, Helv. Chim. Acta **23** (1940), 955.
18) P. Karrer und E. Würgler, Helv. Chim. Acta **26** (1943), 116.
19) P. Karrer und J. Rutschmann, Helv. Chim. Acta **27** (1944), 1684.
20) P. Karrer und E. Jucker, Helv. Chim. Acta **27** (1944), 1695.
21) P. Karrer und E. Jucker, Helv. Chim Acta **28** (1945), 300.
22) P. Karrer und E. Jucker, Helv. Chim. Acta **28** (1945), 427.
23) P. Karrer und E. Jucker, Helv. Chim. Acta **28** (1945), 471.
24) P. Karrer und E. Jucker, Helv. Chim. Acta **28** (1945), 717.
25) P. Karrer und J. Rutschmann, Helv. Chim. Acta **28** (1945), 793.
26) P. Karrer, E. Jucker, J. Rutschmann und K. Steinlin, Helv. Chim. Acta **28** (1945), 1146.
27) P. Karrer und E. Jucker, Helv. Chim. Acta **29** (1946), 229.
28) P. Karrer und E. Jucker, Helv. Chim. Acta **30** (1947), 266.
29) P. Karrer, E. Jucker und K. Steinlin, Helv. Chim. Acta **30** (1947), 531.
30) P. Karrer und E. Jucker, Helv. Chim. Acta **30** (1947), 536.
31) P. Karrer und E. Jucker, Helv. Chim. Acta **30** (1947), 559.
32) H. v. Euler, P. Karrer und E. Jucker, Helv. Chim. Acta **30** (1947), 1159.
33) O. Isler, W. Hubber, A. Ronco und M. Koffer, Helv. Chim. Acta **30** (1947), 1911.
34) P. Karrer, E. Krause-Voith und K. Steinlin, Helv. Chim. Acta **31** (1948), 113.
35) P. Karrer und J. Benz, Helv. Chim. Acta **31** (1948), 1048.
36) P. Karrer und J. Benz, Helv. Chim. Acte **31** (1948), 1607.
37) G. Tappi und P. Karrer, Helv. Chim. Acta **32** (1949), 50.
38) P. Karrer und J. Benz, Helv. Chim. Acta **32** (1949), 232.
39) P. Karrer, K. P. Karanth und J. Benz, Helv. Chim. Acta **32** (1949), 436.
40) P. Karrar, K. P. Karanth und J. Benz, Helv. Chim. Acta **32** (1949), 1036.
41) P. Karrer, D. K. Patel und J. Benz, Helv. Chim. Acta **32** (1949), 1938.
42) P. Karrer und C. H. Eugster, Helv. Chim. Acta **33** (1950), 1433.
43) P. Karrer und C. H. Eugster, Helv. Chim. Acta **33** (1950), 1805.
44) P. Karrer und C. H. Eugster, Helv. Chim. Acta **34** (1951), 28.
45) P. Karrer und E. Leumann, Helv. Chim. Acta **34** (1951), 445.
46) P. Karrer, C. H. Eugster und M. Faust, Helv Chim. Acta **34** (1951), 823.
47) P. Karrer und C. H. Eugster, Helv. Chim. Acta **34** (1951), 1805.
48) C. H. Eugster, C. Garbers und P. Karrer, Helv. Chim. Acta **35** (1952), 1179.
49) A. Polgár and L. Zechmeister, J. Amer. Chem. Soc. **64** (1942), 1856.
50) E. M. Shantz, J. D. Cawley and N. D. Embree, J. Amer. Chem. Soc. **65** (1943), 901.
51) L. Zechmeister and A. Polgár, J. Amer. Chem. Soc. **65** (1943), 1523.
52) L. Zechmeister and A. Polgár, J. Amer. Chem. Soc. **65** (1943), 1528.
53) L. Zechmeister and W. A. Schroeder, J. Amer. Chem. Soc. **65** (1943), 1535.
54) L. Zechmeister, A. L. LeRosen, W. A. Schroeder, A Polgár and L. Pauling, J. Amer. Chem. Soc. **65** (1943), 1940.
55) L. Zechmeister and A. Polgár, J. Amer. Chem. Soc. **66** (1944), 137.
56) L. Zechmeister and A. Polgár, J. Amer. Chem. Soc. **67** (1945), 108.
57) L. Zechmeister und L. v. Cholnoky, Ber. deutsch. chem. Ges. **69** (1936), 422.

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A Quantum Theory of Boson Assemblies, I

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Here we study the temporal evolution of boson assemblies. The equations of the density matrix and of the phase space distribution function are given in the scheme of second quantization. We introduce the velocity operator whose algebraic properties are examined and we intend to reformulate the conventional quantum mechanics in terms of the amplitude operator $\mathcal{R}(x)$ and the velocity operator $v(x)$. The hamiltonian of the system is expressed in terms of these two operators aside from surface effects.

Introduction

To describe assemblies of many equivalent particles, fermions or bosons, as a whole, especially to take the dynamical correlation among particles satisfactorily into consideration and to examine non-equilibrium properties of the system, some reformulations of the conventional interpretation of quantum mechanics have been hoped and proposed by some authors from several points of view. Bloch[1] proposed an idea to describe excited states of many electron atoms by sound wave fields. Tomonaga,[2] applying this theory to many fermion problems, obtained a most complete solution of one dimensional eigenvalue problem, to result in Thomas-Fermi energy as the first term of the power series expansion of the eigenvalue with respect to the coupling constant, the correlation energy appearing as higher order terms. This result has been compared with the higher order perturbation calculus taking many excited fermions and many holes at the neighbourhood of the Fermi surface into consideration. Recently Bohm and Pines[3] have proposed a method of collective description of many fermions as a whole to obtain the theory of plasma oscillations which was also independently found by Kronig.[4] On the other hand, the theory of the density matrix of Husimi[5] was developed by Born and Green[6] and more recently by Irving and Zwanzig[7] to non-equilibrium states introducing the phase space distribution function which was studied by Moyal[8] independently. Our present objective is the non-equilibrium theory of the quantized density matrix for boson assemblies to compute the transformation in terms of quantized operators and to treat the collective behaviour of the assembly as a whole applying the velocity operator. From our point of view, the method of the second quantization has the advantage of the theory of the configuration space in two respects; one is the simplification and the unification of methods used in the conventional theory and the other consists in that the quantized operators appear as field variables.

First we introduce the quantized density matrix of boson assemblies and derive from

it further quantized quantities, such as the phase space distribution function $f(p, q)$, the density operator $\rho(x)$, the current operator $J(x)$ and so on. Commutation relations among these quantities show that the density and the current are the fundamental quantities in the sense that the commutators among them do not give rise to any new quantities, while the commutators of the energy density $E(x)$ with the current and the energy density itself produce new ones such as the stress tensor $\boldsymbol{T}(x)$ and the energy flow $h(x)$ (§ 1). The equation of the quantized density matrix obtained from a prescribed hamiltonian solely determines the temporal evolution of the system in question. We find the transformation function, the so-called S-matrix, as its solution to provide us a complete knowledge of changes with time of the system, and the equation of the phase space distribution function is obtained by a fourier transformation of the density matrix. The solutions of these equations are illustrated by an example of forced harmonic oscillators (§ 2).

Next we introduce the velocity operator and study its algebraic properties. Further consider a function $\Phi(x)$, the velocity potential multiplied by the particle mass m, corresponding to the phase parameter of the configuration wave function. This function $\Phi(x)$ is almost canonically conjugate to the density. The adverb "almost" is used here because this function is not definable unless a projection operator involved in the commutator is set to be zero and the canonical variable does not exist in the strict sense of words (§ 3).

The hamiltonian is now expressed in terms of the velocity and the square root density operator which is introduced quite formally. Such a reformulation involving the velocity operator leads us to easy study of both the classical limit theory and the theory of sound waves given in the next paper.

§ 1. Quantized density matrices

As our object is the boson assembly the quantized density matrix is given by the quantized wave functions subjected to the well-known commutation relations:

$$[\varphi(x), \varphi^*(x')]=\delta(x-x'), \quad [\varphi(x), \varphi(x')]=[\varphi^*(x), \varphi^*(x')]=0, \tag{1·1}$$

and the quantized density matrix is

$$\rho(x, x')=\varphi^*(x')\varphi(x). \tag{1·2}$$

The "mean value" of a one-particle quantity $A(x, x')$, which is really a quantized operator, is given by

$$\langle A\rangle=\int A(x, x')\rho(x', x)dx\,dx'. \tag{1·3}$$

If $A(x, x')$ is obtained by a unitary transformation from a c-number quantity $a(\sigma, \tau)$; thus,

$$A(x, x')=\iint \exp i[\sigma\boldsymbol{P}+\tau\boldsymbol{Q}]a(\sigma, \tau)d\sigma\,d\tau, \tag{1·4}$$

$$\boldsymbol{P}=\frac{\hbar}{i}\frac{\partial}{\partial x}\delta(x-x'), \quad \boldsymbol{Q}=x\delta(x-x'), \tag{1·5}$$

then the "mean value" is expressed by quantities $a(p, q)$ and $f(p, q)$ defined by

$$a(p, q)=\iint \exp i[\sigma p+\tau q]a(\sigma, \tau)d\sigma d\tau\,, \tag{1·6}$$

$$\begin{aligned} f(p, q)&=\left(\frac{1}{2\pi}\right)^6\iiiint M_{\sigma\tau}(x, x')\rho(x', x)\exp[-i\sigma p-i\tau q]dx\,dx'\,d\sigma\,d\tau \\ &=\left(\frac{1}{2\pi}\right)^6\iint m(\sigma, \tau)\exp[-i\sigma p-i\tau q]d\sigma\,d\tau \\ &=\left(\frac{1}{2\pi}\right)^3\int \varphi^*\left(q-\frac{\hbar\sigma}{2}\right)\exp[-i\sigma p]\varphi\left(q+\frac{\hbar\sigma}{2}\right)d\sigma\,, \end{aligned} \tag{1·7}$$

where

$$M_{\sigma\tau}(x, x')=\exp i[\sigma\boldsymbol{P}+\tau\boldsymbol{Q}]=\exp\left[\frac{i}{2}\sigma\boldsymbol{P}\right]\exp[i\tau\boldsymbol{Q}]\exp\left[\frac{i}{2}\sigma\boldsymbol{P}\right], \tag{1·8}$$

$$m(\sigma, \tau)=\int \varphi^*\left(x-\frac{\hbar\sigma}{2}\right)\exp[i\tau x]\varphi\left(x+\frac{\hbar\sigma}{2}\right)dx\,. \tag{1·9}$$

We have

$$\langle A\rangle=\iint a(p, q)f(p, q)dp\,dq\,. \tag{1·10}$$

This is the familiar mean value expression of the classical statistical mechanics regarding $a(p, q)$ as a dynamical quantity and $f(p, q)$ plays the role of the phase space distribution function. To get the explicit forms of A, we assume $a(p, q)$ as follows:

$$a_D(p, q)=\delta(x-q), \qquad \text{density} \tag{1·11}$$

$$a_J(p, q)=\frac{p}{m}\delta(x-q), \quad \text{current} \tag{1·12}$$

$$a_E(p, q)=\frac{p^2}{2m}\,\delta(x-q)+\frac{1}{2}\int G(q, q')\{\rho(q')-\delta(q-q')\}\delta(x-q)dq', \quad \text{energy.} \tag{1·13}$$

Then the "mean values" of these operators are expressed by

$$\langle A_D\rangle=\rho(x)=\varphi^*(x)\varphi(x)\,, \tag{1·14}$$

$$\langle A_J\rangle=J(x)=\frac{\hbar}{2mi}\left\{\varphi^*(x)\frac{\partial\varphi(x)}{\partial x}-\frac{\partial\varphi^*(x)}{\partial x}\varphi(x)\right\}, \tag{1·15}$$

$$\begin{aligned} \langle A_E\rangle=E(x)=&\frac{\hbar^2}{8m}\left\{2\frac{\partial\varphi^*(x)}{\partial x}\cdot\frac{\partial\varphi(x)}{\partial x}-\varphi^*(x)\frac{\partial^2\varphi(x)}{\partial x^2}-\frac{\partial^2\varphi^*(x)}{\partial x^2}\varphi(x)\right\} \\ &+\frac{1}{2}\int G(x, x')\rho(x)\{\rho(x')-\delta(x-x')\}dx'\,, \end{aligned} \tag{1·16}$$

where $\rho(x)$ is the density operator and $J(x)$ is the current operator and $E(x)$ is the energy density operator. The commutation relations between them are given by

$$[\rho(x), \rho(x')]=0\,, \tag{1·17}$$

$$[\rho(x), J(x')]=\frac{i\hbar}{m}\rho(x')\frac{\partial}{\partial x'}\delta(x'-x), \tag{1·18}$$

$$[J_j(x), J_k(x')] = \frac{\hbar}{mi}\left\{J_j(x')\frac{\partial}{\partial x_k}\delta(x-x') + J_k(x)\frac{\partial}{\partial x_j}\delta(x-x')\right\}, \quad (1\cdot19)$$

$$j, k = 1, 2, 3,$$

$$[E(x), \rho(x')] = \frac{\hbar}{i} J(x)\cdot\frac{\partial}{\partial x}\delta(x-x'), \quad (1\cdot20)$$

$$[E(x), J(x')] = \frac{\hbar}{2mi}\left[2\boldsymbol{T}(x)\cdot\frac{\partial}{\partial x}\delta(x-x') + \frac{\partial}{\partial x}\left\{2E(x)\delta(x-x') - \frac{\hbar^2}{4m}\rho(x)\Delta\delta(x-x')\right\} - \rho(x')\frac{\partial}{\partial x'}\delta(x'-x)\int G(x, x'')\{\rho(x'') - \delta(x-x'')\}dx'' - \rho(x)\int G(x, x')\rho(x')\frac{\partial}{\partial x'}\delta(x'-x'')dx''\right], \quad (1\cdot21)$$

$$[E_0(x), E_0(x')] = \frac{\hbar}{i} h(x)\cdot\frac{\partial}{\partial x}\delta(x-x') + \frac{\hbar\partial}{i\partial x}\left\{h(x)\delta(x-x') - \frac{\hbar^2}{4m}J(x)\Delta\delta(x-x')\right\} - \frac{\hbar^2}{4m}\Delta\left\{J(x)\cdot\frac{\partial}{\partial x}\delta(x-x')\right\}, \quad (1\cdot22)$$

where

$$E_0(x) = \frac{\hbar^2}{8m}\left\{2\frac{\partial^*\varphi(x)}{\partial x}\cdot\frac{\partial\varphi(x)}{\partial x} - \varphi^*(x)\Delta\varphi(x) - \Delta\varphi^*(x)\varphi(x)\right\},$$

and the kinetic stress tensor is

$$\boldsymbol{T}(x) = \frac{\hbar^2}{4m}\left[\frac{\partial\varphi^*}{\partial x}\frac{\partial\varphi}{\partial x} + \left(\frac{\partial\varphi^*}{\partial x}\frac{\partial\varphi}{\partial x}\right)^c - \frac{\partial^2\varphi^*}{\partial x\partial x}\varphi - \varphi^*\frac{\partial^2\varphi}{\partial x\partial x}\right], \quad (1\cdot23)$$

$$T_{ik}(x) = T^c_{ki}(x) \text{ etc.},$$

and the kinetic energy flow is

$$h(x) = \frac{\hbar^3}{8m^2 i}\left[2\frac{\partial\varphi^*}{\partial x}\cdot\frac{\partial}{\partial x}\frac{\partial\varphi}{\partial x} - 2\left(\frac{\partial}{\partial x}\frac{\partial\varphi^*}{\partial x}\right)\cdot\frac{\partial\varphi}{\partial x} - \Delta\varphi^*\frac{\partial\varphi}{\partial x} + \frac{\partial\varphi^*}{\partial x}\Delta\varphi + \Delta\frac{\partial\varphi^*}{\partial x}\varphi - \varphi^*\Delta\frac{\partial\varphi}{\partial x}\right]. \quad (1\cdot24)$$

These commutators are available to find the equations of motion. (see note added in proof).

§ 2. Equations of motion

The temporal development of any quantities $A(x)$ is expressed by

$$\frac{\partial A(x)}{\partial t} = \frac{i}{\hbar}\int[H(x'), A(x)]dx' \quad (2\cdot1)$$

where $H(x)$ is the hamiltonian density of the form

$$H(x)=-\frac{\hbar^2}{2m}\frac{\partial\varphi^*}{\partial x}\frac{\partial\varphi}{\partial x}+\frac{1}{2}\int G(x,x')\rho(x)\{\rho(x')-\delta(x-x')\}dx' \qquad (2\cdot2)$$

and $G(x, x')$ is the interaction energy. $H(x)$ is different from the energy density $E(x)$ by a divergence term and the hamiltonian is

$$H=\int H(x)dx=\int E(x)dx\,. \qquad (2\cdot3)$$

The equations of motion as well as the conservation law of density, the conservation law of momentum and the conservation law of energy are given in our foregoing paper[10] for fermion assemblies and the corresponding equations for the present case are quite identical with them so that we need not repeat them here. In this section we ask for the equation of the quantized density matrix, and the equation of the phase space distribution function. After some elementary manipulations one gets the equation of the density matrix in the form

$$\frac{\partial\rho(X,r)}{\partial t}+\frac{\partial}{\partial X}\cdot J(X,r)=\frac{i}{\hbar}\left\{G\left(X-\frac{r}{2},x''\right)-G\left(X+\frac{r}{2},x''\right)\right\}\rho\left(X+\frac{r}{2},x'';X-\frac{r}{2},x''\right)dx'', \qquad (2\cdot4)$$

where

$$X=\frac{x+x'}{2},\quad r=x'-x, \qquad (2\cdot5)$$

$$\rho(X,r)=\varphi^*\left(X-\frac{r}{2}\right)\varphi\left(X+\frac{r}{2}\right),\quad \rho(x,x'';x',x'')=\varphi^*(x')\varphi^*(x'')\varphi(x'')\varphi(x), \qquad (2\cdot6)$$

and

$$J(X,r)=\frac{\hbar}{mi}\frac{\partial}{\partial r}\rho(X,r) \qquad (2\cdot7)$$

is the generalized current operator which is not diagonal with respect to the coordinates. The equation for the phase space distribution function of Wigner is obtained by the fourier transformation of (2·4) to the effect:

$$\frac{\partial f(p,q)}{\partial t}=\frac{1}{(2\pi)^6}\int\frac{\partial m(\tau,\theta)}{\partial t}\exp(-i[\tau p+\theta q])\,d\tau\,d\theta$$
$$=\frac{1}{2}\iint\{S(p,q|\eta,\xi),f(\eta,\xi)\}\,d\eta\,d\xi\,, \qquad (2\cdot8)$$

and

$$\{A,B\}=AB+BA\,, \qquad (2\cdot9)$$

$$S(p,q|\eta,\xi)=\frac{1}{(2\pi)^6}\frac{i}{\hbar}\iint\left[H\left(\eta+\frac{\hbar\theta}{2},\xi-\frac{\hbar\tau}{2}\right)-H\left(\eta-\frac{\hbar\theta}{2},\xi+\frac{\hbar\tau}{2}\right)\right]\exp i[\tau(\eta-p)+\theta(\xi-q)]\,d\tau\,d\theta\,. \qquad (2\cdot10)$$

In the Fock representations in subspaces of 0, 1, 2,……particles the equations (2·4) and

(2·8) are identical with the simultaneous equations of Born-Green and Green. To cut off this infinite chain of the equations one must find the solution of the reduced density matrix with two explicit coordinates with sufficient accuracy. After the reduction the equations become those of one body problem, and this fact will give promise of another approach to the many body problem, other than conventional methods.

For the problem of stationary states we have to find the approximate solution of $\rho(x)$, for, from (2·4) the right side of (2·4) becomes

$$\begin{aligned}&\frac{i}{2\hbar}\int\Big[G\Big(X-\frac{r}{2},x''\Big)-G\Big(X+\frac{r}{2},x''\Big)\Big]\Big[\Big\{\rho\Big(X+\frac{r}{2},X-\frac{r}{2}\Big),\rho(x'')\Big\}\\&\quad-\rho(X,r)\Big(\delta\Big(x''-X-\frac{r}{2}\Big)+\delta\Big(x''-X+\frac{r}{2}\Big)\Big)\Big]\\&=\frac{i}{2\hbar}\int\Big[G\Big(X-\frac{r}{2},x''\Big)-G\Big(X+\frac{r}{2},x''\Big)\Big]\{\rho(X,r),\rho(x'')\}\\&\quad+\frac{i}{2\hbar}\Big[G\Big(X+\frac{r}{2},X-\frac{r}{2}\Big)-G\Big(X-\frac{r}{2},X+\frac{r}{2}\Big)\Big]\rho(X,r).\end{aligned}\tag{2·11}$$

If G is a function of distance $|r|$ only, the last bracket vanishes, hence the equation is similar to the one subject to an external potential;

$$\int G(X,x'')\rho(x'')dx''.\tag{2·12}$$

Aside from the fact that $\rho(x'')$ and $\rho(X,r)$ are not commutative with each other, if $\rho(x)$ is a known parameter, this potential is fixed.

Another equation is derived by the further fourier transformation of equation (2·8) with respect to the center of gravity q. It reads

$$\lambda(p,p')=\Big(\frac{1}{2\pi\hbar}\Big)^3\int f(p,q)\exp\Big[-\frac{i}{\hbar}p'q\Big]dq,\tag{2·13}$$

$$\begin{aligned}&\frac{\partial\lambda(p,p')}{\partial t}+\frac{i}{m\hbar}(p\cdot p')\lambda(p,p')+\frac{i}{2\hbar}\int G(\eta)\Big\{\rho(-\eta),\Big[\lambda\Big(p+\frac{\eta}{2},\eta+p'\Big)\\&\quad-\lambda\Big(p-\frac{\eta}{2},\eta+p'\Big)\Big]\Big\}d\eta=0,\end{aligned}\tag{2·14}$$

which will be available to the theory in the momentum space. To get greater familiarity with these equations we consider an example of harmonic oscillators subject to the external potential $xF(t)$.

Example: Forced oscillators.

Let the external force be $F(t)$. Then the equation of the density matrix for the one dimensional forced oscillator with frequency Ω becomes

$$\frac{\partial\rho(x,r)}{\partial t}+\frac{\hbar}{mi}\frac{\partial}{\partial x}\frac{\partial}{\partial r}\rho(x,r)+\frac{i}{\hbar}m\Omega^2xr\rho(x,r)+\frac{i}{\hbar}F(t)r\rho(x,r)=0.$$

Applying the transformation

$$t'=t, \quad x'=x-X(t), \quad \ddot{X}(t)+\Omega^2 X(t)+\frac{F(t)}{m}=0,$$

and

$$\rho(x, r)\exp\left[\frac{i}{\hbar}m\dot{X}(t)r\right]\rho'(x', r),$$

the equation for $\rho'(x', r)$ takes the form

$$\frac{\partial\rho'(x', r)}{\partial t'}+\frac{\hbar}{mi}\frac{\partial}{\partial x'}\frac{\partial}{\partial r}\rho'(x', r)+\frac{i}{\hbar}m\Omega^2 x'r\rho'(x', r)=0.$$

This is the well-known equation of the harmonic oscillator. Since we have interest in the transformation function, we assume its form as

$$U'(x', r)=\frac{m\Omega}{2\pi\hbar}\exp\frac{i}{\hbar}[a(t)x'r+b(t)x'+c(t)r+d(t)].$$

Then one finds the simultaneous equations*)

$$\dot{a}(t)+\frac{a(t)^2}{m}+m\Omega^2=0,$$

$$\dot{b}(t)+\frac{1}{m}a(t)b(t)=0, \quad \dot{c}(t)+\frac{1}{m}a(t)c(t)=0,$$

$$\dot{d}(t)+\frac{\hbar}{i}\frac{a(t)}{m}+\frac{1}{m}b(t)c(t)=0,$$

whose solutions become

$$a(t)=m\Omega\cot\Omega t,$$

$$c(t)=-m\Omega\frac{x''}{\sin\Omega t}, \quad b(t)=-m\Omega\frac{r''}{\sin\Omega t},$$

$$d(t)=-\frac{\hbar}{i}\log\sin\Omega t+m\Omega x''r''\cot\Omega t$$

where x'' and r'' are integration constants. Hence the transformation function of the density matrix $U(x, r\,;\, x'', r'')$ becomes

$$U(x, r\,;\, x'', r'')=\frac{m\Omega}{2\pi\hbar\sin\Omega t}\exp\frac{i}{\hbar}m\Omega\left[xr\cot\Omega t-\frac{x''r+r''x}{\sin\Omega t}\right.$$
$$\left.+x''r''\cot\Omega t+\frac{\dot{X}(t)}{\Omega}r\right].$$

The transformation function of the phase space distribution function is obtained by the fourier transformation of U with respect to r and r'' as follows:

$$K(p, x\,;\, p', x')=\frac{1}{2\pi\hbar}\iint U(x, r\,;\, x', r')\exp\frac{i}{\hbar}[r'p'-rp]\,dr\,dr'$$
$$=\delta\left(x'+\frac{p-m\dot{X}(t)}{m\Omega}\sin\Omega t-\overline{x-X(t)}\cos\Omega t\right)$$
$$\times\delta(p'-\overline{p-m\dot{X}(t)}\cos\Omega t-m\Omega\overline{x-X(t)}\sin\Omega t)$$

* The author is indebted much to Professor Husimi for showing him the manuscript before the publication.

which satisfies the equation of the phase space distribution function.

$$\frac{\partial f(p,x)}{\partial t}+\frac{p}{m}\frac{\partial}{\partial x}f(p,x)-m\Omega^2 x\frac{\partial}{\partial p}f(p,x)-F(t)\frac{\partial}{\partial p}f(p,x)=0.$$

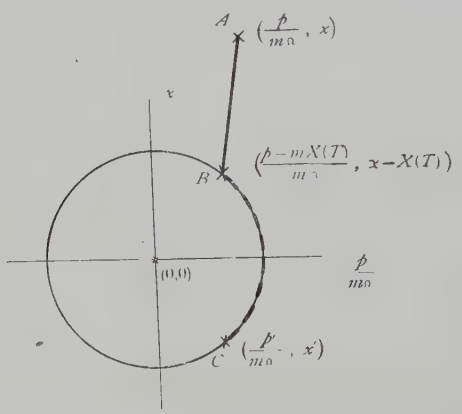

Fig. 1. The phase point $(p/m\Omega, x)$ at the initial time, $t=0$, is shifted to the point $(p'/m\Omega, x')$ at the final time, $t=T$. The transformation is divided into two processes; from A to B the center of the wave packet moves along the classical path and from B to C the motion is subject to the transformation of the free harmonic oscillator with frequency Ω.

§ 3. Velocity operator

We introduce the velocity operator of the quantized wave field by the phase functions defined by[11]

$$\varphi^*(x)=R(x)\Psi^*(x), \tag{3·1}$$

$$\varphi(x)=\Psi(x)R(x), \tag{3·2}$$

$$\varphi^*(x)\varphi(x)=R(x)^2=\rho(x), \quad R(x): \text{real}, \tag{3·3}$$

and the velocity operator is expressed by

$$v(x)=\frac{\hbar}{2mi}\left\{\Psi^*(x)\frac{\partial\Psi(x)}{\partial x}-\frac{\partial\Psi^*(x)}{\partial x}\Psi(x)\right\}, \tag{3·4}$$

and the current operator takes the form

$$J(x)=R(x)v(x)R(x). \tag{3·5}$$

Here we examine some algebraic properties of the velocity operator from the commutation relations

$$[\rho(x'),\ \Psi^*(x)]=\delta(x-x')\Psi^*(x), \tag{3·6}$$

$$[\rho(x'),\ \Psi(x)]=-\delta(x-x')\Psi(x). \tag{3·7}$$

One gets the commutation relation between the velocity and the density:

$$[\rho(x'),\ v(x)]=-\frac{\hbar}{mi}\{1-\varepsilon(x)\}\frac{\partial}{\partial x}\delta(x-x'), \tag{3·8}$$

in which $\varepsilon(x)=[\Psi(x), \Psi^*(x)]$ is a projection operator having value unity if the eigenvalue of $\rho(x)$ is zero, and value zero if the eigenvalue of $\rho(x)$ is not zero. Further we get the commutation relation between the velocity components in the form

$$[v_j(x), v_k(x')]=-\frac{\hbar}{mi}\left[\{\mathrm{rot}\, v(x)\}_{jk}+\frac{1}{2}\left\{\frac{\partial\varepsilon(x)}{\partial x}\times v(x)\right\}_{jk}-\frac{1}{2}\left\{v(x)\times\frac{\partial\varepsilon(x)}{\partial x}\right\}_{jk}\right]\delta_{x,x'},$$
$$j, k=1, 2, 3. \tag{3·9}$$

Here we confine ourselves to a subspace corresponding to the eigenvalue $\varepsilon(x)=0$. According to the convention, field quantities of continuous parameters running over the lattice points (l, m, n) in the coordinate space. Let the real and the imaginary parts of the wave function $\varphi(x)$ be $q(x)/\sqrt{2}$ and $p(x)/\sqrt{2}$ respectively and the corresponding quantities of discrete parameter by $q(l, m, n)$ and $p(l, m, n)$ satisfying the commutation relations:

$$[p(l, m, n), q(l', m', n')]=\frac{1}{i}\delta_{l,l'}\delta_{m,m'}\delta_{n,n'}, \tag{3·10}$$

$$[p(l, m, n), p(l', m', n')]=[q(l, m, n), q(l', m', n')]=0. \tag{3·11}$$

The particle number operator $N(l, m, n)$ at (l, m, n) is expressed by

$$N(l, m, n)=\frac{1}{2}p(l, m, n)^2+\frac{1}{2}q(l, m, n)^2-\frac{1}{2}. \tag{3·12}$$

We consider a subspace of the operator $N(l, m, n)$ spanned by the eigenfunctions $\chi_\mu(l, m, n)$ of the eigenvalues $\mu(l, m, n)$ which are not smaller than $M-1$. To our regret such a subspace is not invariant in the sense that an operator A, a product of the phase function Ψ^* and Ψ, may shift the eigenfunction out of such a subspace to the wider one. For instance, matrix elements of operators involving $\varepsilon(x)$, in the representation where $N(l, m, n)$ is diagonal, become

$$[\varepsilon(l, m, n)]_{\mu\nu}=\delta_{\mu,0}\delta_{\nu,0}, \tag{3·13}$$

$$[\Psi^*(l, m, n)\varepsilon(l, m, n)\Psi(l, m, n)]_{\mu\nu}=\delta_{\mu-1,0}\delta_{\nu-1,0}, \tag{3·14}$$

$$[\underbrace{\Psi^*(l, m, n)\cdots\Psi^*(l, m, n)}_{\alpha\text{—factors}}\varepsilon(l, m, n)\underbrace{\Psi(l, m, n)\cdots\Psi(l, m, n)}_{\beta\text{—factors}}]_{\mu\nu}=\delta_{\mu-\alpha,0}\delta_{\nu-\beta,0}. \tag{3·15}$$

Hence if the eigenvalues μ and ν are larger than a finite value M which is sufficiently larger than α and β, that may occur, these operators involving the projection operator ε may be regarded as zero. Under such circumstances, the wave functions φ^*, φ and the density $\rho(x)$ are defined by dividing the quantities p, q, and N by the small volume element Δ as follows:

$$\varphi(x)=\lim_{\Delta\to 0}\frac{1}{\sqrt{2\Delta}}[q(l, m, n)+ip(l, m, n)], \tag{3·16}$$

$$\varphi^*(x)=\lim_{\Delta\to 0}\frac{1}{\sqrt{2\Delta}}[q(l, m, n)-ip(l, m, n)], \tag{3·17}$$

$$\rho(x)=\lim_{\Delta\to 0}\frac{1}{\Delta}N(l, m, n), \tag{3·18}$$

and

$$x=(\delta l, \delta m, \delta n),\ \Delta=\delta^3.$$

Strictly speaking, one can discriminate the quantum states not by the eigenvalues of the density but by the eigenvalues of the limit function of the particle number at (l, m, n) ; $N(l, m, n)$. The above-mentioned subspace designated by the arbitrarily chosen lower limit of these eigenvalues makes the basis of a classical-limit theory in the following paper. So long as we operate within such a space the phase functions and their derivatives become commutative with one another, and hence the velocity operator may be regarded as irrotational due to the commutation relation (3·9) and may be expressed in the form

$$v(x)=\frac{1}{m}\operatorname{grad}\Phi(x). \tag{3·19}$$

Further as seen from the commutation relation (3·8), the phase parameter $\Phi(x)$ is canonically conjugate to the density $\rho(x)$:

$$[\rho(x'), \Phi(x)]=i\hbar\delta(x-x'). \tag{3·20}$$

§ 4. Hamiltonian in terms of the new variables

The total energy of the system is given by the energy expression given in § 1. We write this energy density in terms of the square root density $R(x)$ and the velocity $v(x)$ and the projection operator $\varepsilon(x)$ as follows :

$$\begin{aligned}E(x)=&\frac{m}{2}R(x)v(x)^2R(x)+\frac{\hbar^2}{4m}\{|\operatorname{grad}R(x)|^2-R(x)\Delta R(x)\}\{\mathbf{1}-\varepsilon(x)\}\\&+\frac{\hbar}{4i}\{R(x)v(x)\cdot\operatorname{grad}R(x)-\operatorname{grad}R(x)\cdot v(x)R(x)\}\\&+\frac{1}{2}\rho(x)\int G(x, x')\{\rho(x')-\delta(x-x')\}dx'\\&+E_{\mathrm{vac}}(x),\end{aligned} \tag{4·1}$$

and

$$\begin{aligned}E_{\mathrm{vac}}(x)=&\frac{\hbar^2}{8m}R(x)\left\{\frac{\partial^2\varepsilon(x)}{\partial x^2}+\left|\frac{\partial\varepsilon(x)}{\partial x}\right|^2\right\}R(x)+\frac{\hbar}{4i}R(x)\left\{\frac{\partial\varepsilon(x)}{\partial x}\cdot v(x)\right.\\&\left.-v(x)\cdot\frac{\partial\varepsilon(x)}{\partial x}\right\}R(x),\end{aligned} \tag{4·2}$$

where the derivative of the projection operator, which is a discontinuous function, is quite formal. The integration of $E_{\mathrm{vac}}(x)$ over the whole space amounts to

$$\int E_{\mathrm{vac}}(x)dx=\frac{\hbar^2}{4m}\int\varepsilon(x)\left|\frac{\partial R(x)}{\partial x}\right|^2dx+\frac{\hbar^2}{8m}\int\left|\frac{\partial\varepsilon(x)}{\partial x}\right|^2\rho(x)dx. \tag{4·3}$$

The first term of the right side cancels the same term in the expression (4·1). The

second term is appreciable merely at the boundary of the zero density region, therefore it represents a sort of surface effects, aside from which the hamiltonian becomes

$$H=\int\left[\frac{m}{2}R(x)v(x)^2R(x)+\frac{\hbar^2}{2m}\left|\frac{\partial R(x)}{\partial x}\right|^2+\frac{\hbar}{4i}\left\{R(x)v(x)\cdot\frac{\partial R}{\partial x}-\frac{\partial R(x)}{\partial x}\cdot v(x)R(x)\right\}\right]dx+\frac{1}{2}\iint G(x,x')\rho(x)\{\rho(x')-\delta(x-x')\}dx\,dx'. \tag{4·4}$$

In terms of the fourier coefficients of the quantities this expression turns out into

$$\begin{aligned}H=&\frac{m}{2}\sum_k\sum_{k'}\sum_l R(l-k-k')v(k)v(k')R(-l)\\&+\frac{\hbar}{2}\sum_k\sum_{k'}(k'-k)R(k)v(-k-k')R(k')\\&+\frac{\hbar^2}{2m}\sum_k k^2R(k)R(-k)+\frac{1}{2}\sum_{k\neq 0}G(k)\rho(k)\rho(-k)\\&+\frac{1}{2}G(0)\rho(0)^2-\frac{1}{2}G_0\rho(0),\end{aligned} \tag{4·5}$$

where

$$G(k)=G(-k)=\frac{1}{V^2}\iint G(x-x')\exp[-ik(x-x')]dx\,dx', \tag{4·6}$$

$$G_0=\int G(x-x')\delta(x-x')dx', \tag{4·7}$$

V: volume of box

and

$$R(k)=\frac{1}{\sqrt{V}}\int_V R(x)\exp[-ikx]dx,\quad v(k)=\int_V v(x)\exp[-ikx]dx. \tag{4·8}$$

The author would like to thank Professor Tomonaga and Professor Husimi for their valuable discussions. He also thanks the financial aid of the Yukawa Fund.

Appendix I

The transport equations are obtained by developing the equations of density matrix in the power series with respect to the relative coordinate r. The zero order terms read

$$\frac{\partial\rho(x)}{\partial t}+\operatorname{div}J(x)=0, \tag{A·1·1}$$

$$J(x)=\frac{\hbar}{mi}\left[\frac{\partial}{\partial r}\rho(X,r)\right]_{r=0}, \tag{A·1·2}$$

which is the equation of the density conservation law. The second terms become

$$m\frac{\partial J(x)}{\partial t}+\operatorname{div}\boldsymbol{T}(x)+\rho(x)\operatorname{grad}\int G(x,x')\{\rho(x')-\delta(x-x')\}dx'=0, \tag{A·1·3}$$

$$\boldsymbol{T}(x)=m\Big(\frac{\hbar}{mi}\Big)^2\Big[\frac{\partial}{\partial r}\frac{\partial}{\partial r}\rho(X,r)\Big]_{r=0}, \qquad (A\cdot1\cdot4)$$

which represents the momentum conservation law. The third-order terms read

$$\frac{\partial E_0(x)}{\partial t}+\operatorname{div}h(x)+J(x)\cdot\operatorname{grad}\int G(x,x')\{\rho(x')-\delta(x-x')\}dx' + \frac{\hbar}{2mi}\rho(x)\Big[\frac{\partial^2 G(r)}{\partial r^2}\Big]_{r=0}=0, \qquad (A\cdot1\cdot5)$$

$$E_0(x)=\frac{m}{2}\Big(\frac{\hbar}{mi}\Big)^2\Big[\frac{\partial^2}{\partial r^2}\rho(X,r)\Big]_{r=0}, \qquad (A\cdot1\cdot6)$$

$$h(x)=\frac{m}{2}\Big(\frac{\hbar}{mi}\Big)^3\Big[\frac{\partial}{\partial r}\frac{\partial^2}{\partial r^2}\rho(X,r)\Big]_{r=0}, \qquad (A\cdot1\cdot7)$$

which is the transport equation of the kinetic energy density. The equation of the total energy density is expressed by

$$\frac{\partial E}{\partial t}+\operatorname{div}h(x)+J(x)\cdot\operatorname{grad}\int G(x,x')\rho(x')dx'+\frac{1}{2}\operatorname{div}J(x)\int G(x,x')\rho(x')dx' + \frac{1}{2}\rho(x)\int G(x,x')\operatorname{div}J(x')dx'+\frac{\hbar}{2mi}\rho(x)\Big[\frac{\partial^2 G(r)}{\partial r^2}\Big]_{r=0} - J(x)\cdot\Big[\frac{\partial G(r)}{\partial r}\Big]_{r=0}-\frac{1}{2}\operatorname{div}J(x)G(0)=0. \qquad (A\cdot1\cdot8)$$

These equations are identical with those ones given in Paper I and will be given in terms of density operators and velocity operators in the next paper.

Appendix II *Generating function of phase space eigen-functions*

Moyal introduced the so-called phase space eigenfunction defined by

$$f_{jk}(p,q)=\frac{1}{(2\pi)^3}\int\overline{\Psi_j(q-\tfrac{1}{2}\hbar\tau)}\Psi_k(q+\tfrac{1}{2}\hbar\tau)\exp[-i\tau p]d\tau, \qquad (A\cdot2\cdot1)$$

where $\overline{\Psi_j(q)}$, $\Psi_j(q)$ constitute a complete-orthogonal set. We introduce the generating function of f_{jk} defined by

$$G_{s,t}(p,q)=\sum_{m,n}\alpha(m)\beta(n)s^m t^n f_{mn}(p,q), \qquad (A\cdot2\cdot2)$$

in which $\alpha(m)$, $\beta(n)$ are normalization factors. As an example we consider the one dimensional harmonic oscillator with frequency Ω. Setting

$$\Psi_m(q)=\frac{(-i)^m}{\sqrt{2\pi m!}}\Big(\frac{\alpha}{\pi}\Big)^{1/4}e^{(\alpha/2)q^2}\int_{-\infty}^{\infty}u^m\exp\Big[-\frac{u^2}{2}+i\sqrt{2\alpha}qu\Big]du, \qquad (A\cdot2\cdot3)$$

$$\alpha=\frac{m\Omega}{\hbar},\quad \alpha(m)=\frac{1}{\sqrt{m!}},\quad \beta(n)=\frac{1}{\sqrt{n!}},$$

the generating function takes the form

$$G_{s,t}(p,q)=\frac{1}{\pi\hbar}\exp\left[-aq^2-\frac{p^2}{a\hbar^2}-ts+\sqrt{2a}\,(s+t)q+i\sqrt{\frac{2}{a}}\,(s-t)\frac{p}{\hbar}\right]. \tag{A·2·4}$$

Taking the complex conjugate and exchanging s and t one finds that this expression remains invariant. This fact is an evidence of the hermite character of f_{jk}. For instance,

$$f_{1,0}(p,q)=\frac{\sqrt{2a}}{\pi\hbar}\left[q+i\frac{p}{m\Omega}\right]\exp\left[-aq^2-\frac{p^2}{a\hbar^2}\right]=\overline{f_{0,1}(p,q)}. \tag{A·2·5}$$

Letting

$$Q=\frac{2}{\hbar\Omega}\left[m\Omega^2+\frac{p^2}{m}\right],\quad \sqrt{2a}\,X+i\sqrt{\frac{2}{a}}\,\frac{p}{\hbar}=s',\quad \sqrt{2a}\,X-i\sqrt{\frac{2}{a}}\,\frac{p}{\hbar}=t', \tag{A·2·6}$$

one obtains

$$\begin{aligned}G_{s',t'}(p,q)&=\frac{1}{\pi\hbar}\exp\left[-aq^2-\frac{p^2}{a\hbar^2}-\frac{s't'}{Q}+s'+t'\right]\\&=\frac{1}{\pi\hbar}\exp\left[-aq^2-\frac{p^2}{a\hbar^2}\right]\sum_{m,n}c(m,n,Q)s'^m t'^n,\end{aligned} \tag{A·2·7}$$

where $c(m,n,Q)$ is called Chalier's polynomial. Hence the phase space eigenfunction $f_{m,n}(p,q)$ is expressed by Chalier's polynomial as follows:

$$\begin{aligned}f_{m,n}(p,q)=\frac{c(m,n,Q)}{\pi\hbar}&\frac{[\sqrt{2a}\,q+i\sqrt{a/2}\cdot p/\hbar]^m[\sqrt{2a}\,q-i\sqrt{a/2}\cdot p/\hbar]^n}{(m!\,n!)^{1/2}}\\&\cdot\exp\left[-dq^2-\frac{p^2}{a\hbar^2}\right].\end{aligned} \tag{A·2·8}$$

Note added in proof:

(1) All the commutation relations (1.18—1.22) are readily obtained from the commutation relation between the two density matrices:

$$[\rho(x,r),\rho(x',r')]=\rho\left(x+\frac{r'}{2},R\right)\delta\left(x-x'+\frac{R}{2}\right)-\rho\left(x-\frac{r'}{2},R\right)\delta\left(x'-x+\frac{R}{2}\right),$$

where $R=r+r'$. (see § 7 and Appendix I).

(2) We shall study in the next paper the behavior of the individual particle embedded in the assembly. The interaction of the individual particle with the remainder of the assembly turns out to be that of the individual particle with a sound field, which gives rise to the self-energy of the individual particle and the Møller interaction between particles.

References

1) F. Bloch, Helv. Phys. Acta **7** (1934), 385.
2) S. Tomonaga, Prog. Theor. Phys. **5** (1950), 544.
3) D. Pines and D. Bohm, Phys. Rev. **85** (1952), 338.
4) R. L. Kronig (and Korringa), Physica **10** (1943), 406, 800; **15** (1949), 667.
5) K. Husimi, Proc. Phys. Math. Soc. Japan **22** (1940), 264.
6) M. Born and H. S. Green, Proc. Roy. Soc. **A191** (1947), 138.
7) J. H. Irving and R. W. Zwanzig, J. Chem. Phys. **19** (1951), 1173.
8) J. E. Moyal, Proc. Camb. Phil. Soc. **45** (1949), 99.
9) T. Nishiyama, Prog. Theor. Phys. **6** (1951), 366.
10) H. S. Green, J. Chem. Phys. **19** (1951), 955.
11) T. Nishiyama, Prog. Theor. Phys. **7** (1952), 417.

Letters to the Editor

Magnetic Moment of Li^6

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Of odd-odd nuclei, their nuclear spins and magnetic moments are measured only for stable nuclei, Li^6, Be^{10}, N^{14}, V^{50} and for long-lived beta active nuclei, Na^{22}, K^{40}. Their magnetic moments are well explained by Feenberg's j-j coupling model, while in the case of Li^6 the value calculated by this model shows deviation from the experimental value by about 25%. To explain the deviation we have assumed tensor interaction between $2p$ proton and $2p$ neutron, which will result in the admixture of D-state to the S-ground state. This model is also introduced by Hitchcock[1] to investigate the excited levels of Li^6.

We take for the wave function Ψ the linear combination of ^3S and ^3D waves:

$$\Psi = A\psi_S + B\psi_D, \quad A^2 + B^2 = 1$$

with

$$\psi = {}^3Z(j_1, j_2, m_1, m_2;\ l_1, l_2) \times r_1 r_2\, \varphi(r_1, r_2) \cdot {}^1(\tau)_0$$

and for the interaction between nucleons the potential

$$V(r) = J(r)(1 + bS_{12})$$

where r is the relative distance of proton and neutron in $2p$ orbit and S_{12} the well known tensor operator. The matrix elements which determine the D-state probability, are obtained by performing the integration on the angular parts of ψ_S and ψ_D, and summation with respect to spin and isotopic spin. For the radial parts of wave functions and the nuclear potential, we have assumed the Gauss type function:

$$J(r) = J_0 \exp(-ar^2),$$

and

$$|\varphi(r, R)|^2 = \exp(-a\sigma(4R^2 + r^2)) \cdot N^2$$

with

$$\boldsymbol{R} = \frac{1}{2}(\boldsymbol{r}_1 + \boldsymbol{r}_2), \quad \boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2,$$

$\boldsymbol{r}_1$, $\boldsymbol{r}_2$ being neutron and proton coordinates with respect to the centre of nucleus. N is normalization factor. J_0, a and σ are determined so as to fit the nuclear dimensions of Li^6. However, the final results do not depend on J_0 and a in our choice and thus, to obtain the amount of the D-state admixture, we have only to know the value of b and σ. The ratio b of the potential strength in central and non-central parts is taken from the neutron-proton forces as 0.7. The calculated values for D-state probability, $P(D)$, and the magnetic moment as the function of σ are given in the Table.

Table. D-state probability and magnetic moment

	0.7	0.6	0.5	0.4
$P(D)$ (%)	6	7.5	7.8	7.3
μ_{cal}	0.830	0.818	0.815	0.819

The above figures agree well with the experimental value, 0.821 and do not depend much on the variation of σ. The agreement may be attributed to the simple structure of Li^6 and the weak coupling between alpha-core and $2p$ nucleons.

In the above discussion, we have employed the Gaussian function for both nuclear potential and the radial parts of wave functions, and this might not give quantitatively correct values. To check the validity we have estimated the order of magnitude of the first excited level, assuming $J_0 = 27$ Mev for the potential strength, which is obtained from the deuteron binding energy. The estimated separation between ground state and the first excited state is about 2.6 Mev for $\sigma = 0.6$. This is compatible with the observed excited level.

1) A. J. M. Hitchcock, Proc. Phys. Soc. **65** (1952), 661.

The Equation of Motion of a Spinning Particle in a Meson Field

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The divergence difficulties associated with the self-force in a field theory, recently led Wheeler and Feynman[1] to revive the theory of "Action at a distance", previously studied by Fokker and others. By incorporating in it the conception of "complete absorption" they succeeded in obtaining the equation of motion of a point particle in an electromagnetic field, which described the reaction of the radiation correctly. Kanazawa[2] and Havas[3] have extended Wheeler and Feynman's theory to derive the equation of motion of a nucleon having a mesic charge. We shall in the present note further develop the theory to obtain the equations of motion of a spinning particle, with spin moment g moving in a neutral meson field.

We start with the variation principle which, for vector meson field, makes the action given by

$$J=\sum_i\int T_i d\tau_i+\sum_{i<k} g_i g_k \frac{\partial}{\partial z_i^\mu}\frac{\partial}{\partial z_{k\nu}} \iint G(z_i-z_k)\, S_{i\rho}^{\mu} S_{k\nu}^{\rho}\, d\tau_i\, d\tau_k \qquad (1)$$

at extremum.

Here the metric tensor $g_{\mu\nu}$ is taken as $g_{00}=-g_{11}=-g_{22}=-g_{33}=1$, and the velocity of light $c=1$; τ_i, $z_{i\mu}$, and $S_{i\mu\nu}$ denote respectively the proper time, the coordinates and spin of the particle "i" and T_i is the angular momentum tensor.

$G(s)$ is the Green's function satisfying the equation,

$$\left(\frac{\partial^2}{\partial x_\mu \partial x^\mu}+\lambda^2\right)G(s) =4\pi\delta(s_0)\,\delta(s_1)\,\delta(s_2)\,\delta(s_3) \qquad (2)$$

where

$$s^2=(x_\mu-z_\mu)(x^\mu-z^\mu)\;;\quad \lambda=M/\hbar,$$

$$M=\text{rest mass of meson.} \qquad (3)$$

We define

$$\phi_{k\nu}(x)=g_k\frac{\partial}{\partial x_\mu}\int_{-\infty}^{\infty} S_{k\mu\nu}(\tau_k)\,G(s_k)\,d\tau_k \qquad (4)$$

and

$$G_{k\mu\nu}(x)=\partial\phi_{k\nu}(x)/\partial x^\mu-\partial\phi_{k\mu}(x)/\partial x^\nu. \qquad (5)$$

Now giving a small rotation $\delta\Omega_{a\rho\nu}$ to particle "a" and remembering

$$\delta T_a=\frac{1}{2}I_a S_{a\mu\nu}\delta\omega_a^{\mu\nu}\;;\quad \delta\omega_{a\mu\nu}=\frac{d}{d\tau_a}(\delta\Omega_{a\mu\nu}) \qquad (6)$$

we obtain the equations of motion after applying the condition of "complete absorption", and $S_{\mu\nu}v^\nu=0$,

$$I_a(\dot{S}_{a\mu\nu}+v_{a\mu}\dot{S}_{a\nu\rho}v_a^\rho-\tau'^{+}_{a\nu}\dot{S}_{a\mu\rho}\tau'^{\rho}_{a}) =g_a\left[S_{a\mu}^{\rho}D^{\mathrm{rad}}_{a\rho\nu}\right]_- +g_a\sum_{k\neq a}\left[S_{a\mu}^{\rho}(G^{\mathrm{ret}}_{k\rho\nu} -G^{\mathrm{ret}}_{k\rho\sigma}\tau'^{\sigma}_{a}\tau'_{a\nu})\right]_-.$$

The minus sign after the square bracket denotes that the terms inside the bracket with μ and ν interchanged are to be subtracted and the dots indicate differentiation with respect to the proper time.

We have used the abbreviation

$$D_{\mu\nu}=G_{\mu\nu}-G_{\mu\rho}v^\rho v_\nu. \qquad (8)$$

The equations obeyed by the potentials and the field strengths are easily obtained from (2), (4) and (5);

$$\left.\begin{aligned}\left(\frac{\partial^2}{\partial x_\mu\partial x^\mu}+\lambda^2\right)\phi_{k\nu}(x)&=4\pi\frac{\partial}{\partial x_\rho}\sum_{k\rho\nu}(x),\\ \partial\phi_{k\mu}(x)/\partial x_\mu&=0\end{aligned}\right\} \qquad (9)$$

and

$$\frac{\partial G_{k\mu\nu}(x)}{\partial x_\mu}+\lambda^2\phi_{k\nu}(x)=4\pi\frac{\partial}{\partial x_\mu}\sum_{k\mu\nu}(x) \qquad (10)$$

where dipole density tensor $\Sigma_{k\mu\nu}$ is defined as

$$\Sigma_{k\mu\nu}(x)=g_k\int_{-\infty}^{\infty}S_{k\mu\nu}(\tau_k)\delta^4(x_\rho-z_\rho(\tau_k))d\tau_k. \tag{11}$$

It can be further verified that the potentials (4), and consequently the fields (5), are given by half the sum of the retarded and the advanced potentials, and fields of the particle k.

The evaluation of the fields $G^{\rm rad}_{a\mu\nu}(z_a)=\frac{1}{2}\{G^{\rm ret}_{a\mu\nu}(z_a)-G^{\rm adv}_{a\mu\nu}(z_a)\}$ on the world line of the particle "a" can be carried out by Riesz method of analytical continuation[4]. We obtain thus

$$\begin{aligned}D^{\rm rad}_{a\mu\nu}(z_a)=&g_a\Big\{\frac{2}{3}S_{a\mu\nu}(\dot v_a\ddot v_a)+\frac{2}{3}\dot S_{a\mu\nu}\dot v_a^2\\&+\frac{2}{3}\dddot S_{a\mu\nu}-\Big[\frac{2}{3}\dddot S_{a\mu\rho}v_a^\rho v_{a\nu}+\frac{4}{3}\dot S_{a\mu\rho}\dot v_a^\rho v_{a\nu}\dot v_a^2\\&+\frac{2}{3}\dot S_{a\mu\rho}v_a^\rho\ddot v_{a\nu}+\frac{4}{3}\ddot S_{a\mu\rho}\dot v_a^\rho v_{a\nu}\\&+\frac{2}{3}\dot S_{a\mu\rho}\dot v_a^\rho\dot v_{a\nu}\Big]_-+\lambda^2\Big[\frac{1}{2}\dot S_{a\mu\nu}-\dot S_{a\mu\rho}v_a^\rho v_{a\nu}\Big]_-\\&+\bar G_{a\mu\nu}-\bar G_{a\mu\rho}v_a^\rho v_{a\nu},\end{aligned} \tag{12}$$

where

$$\begin{aligned}\bar G_{a\mu\nu}=&g_a\lambda^2\Big\{\int_{-\infty}^{\tau}S_{a\mu\nu}\frac{J_2(\lambda s)}{s^2}d\tau_a\\&-\int_{\tau}^{\infty}S_{a\mu\nu}\frac{J_2(\lambda s)}{s^2}d\tau_a\Big\}\\&-g_a\frac{\lambda^3}{2}\Big\{\int_{-\infty}^{\tau}[s_{a\mu}s_a^\rho S_{a\rho\nu}]_-\frac{J_3(\lambda s)}{s^3}d\tau_a\\&-\int_{\tau}^{\infty}[s_{a\mu}s_a^\rho S_{a\rho\nu}]_-\frac{J_3(\lambda s)}{s^3}d\tau_a\Big\}.\end{aligned} \tag{13}$$

The equations of motion obtained from (7), (12) and (13) differ from the equations of the field theory by the additional terms in (13) containing the integrals over τ.

Similarly the equations of a spinning particle in a scalar meson field can be obtained from the variation of the action given by

$$J=\sum_i\int T_i d\tau_i+\sum_{i<k}g_ig_k\frac{\partial}{\partial z_i^\rho}\frac{\partial}{\partial z_{k\sigma}}$$

$$\times\iint G(z_i-z_k)\,S_i^\rho S_{k\sigma}d\tau_i d\tau_k \tag{14}$$

with $$\delta T_i=\frac{1}{2}I_i\epsilon_{\mu\nu\rho\sigma}\delta\omega_i^{\mu\nu}v_i^\rho S_i^\sigma \tag{15}$$

where $\epsilon_{\mu\nu\rho\sigma}$ is antisymmetric in all the indices and $\epsilon_{0123}=1$. Defining again,

$$\phi_k(x)=g_k\frac{\partial}{\partial x_\mu}\int_{-\infty}^{\infty}G(s_k)\,S_{k\mu}(\tau_k)\,d\tau_k \tag{16}$$

and $$G_{k\mu}(x)=\partial\phi_k(x)/\partial x^\mu \tag{17}$$

and further putting $S_\mu v^\mu=0$, the corresponding equations of motion in a scalar meson field are obtained as,

$$\begin{aligned}I_a\,\epsilon_{\mu\nu\rho\sigma}v_a^\rho\dot S_a^\sigma=&g_a[G^{\rm rad}_{a\mu}S_{a\nu}-G^{\rm rad}_{a\alpha}v_a^\alpha S_{a\mu}v_{a\nu}]_-\\&+g_a\sum_{k\neq a}[G^{\rm ret}_{k\mu}S_{a\nu}-G^{\rm ret}_{k\alpha}v_a^\alpha S_{a\mu}v_{a\nu}]_-\end{aligned} \tag{18}$$

where

$$\begin{aligned}G^{\rm rad}_{a\mu}(z_a)=&g_a\Big\{\frac{1}{3}S_{a\mu}(\dot v_a\ddot v_a)+\frac{1}{3}\dot S_{a\mu}\dot v_a^2\\&+\frac{1}{3}\dddot S_{a\mu}-\Big(\frac{2}{3}\dot S_{a\rho}v_a^\rho\ddot v_{a\mu}+\frac{4}{3}\ddot S_{a\rho}v_a^\rho\dot v_{a\mu}\\&+\frac{2}{3}\dot S_{a\rho}\dot v_a^\rho\dot v_{a\mu}+\dddot S_{a\rho}v_a^\rho v_{a\mu}+\dot S_{a\rho}v_a^\rho v_{a\mu}\dot v_a^2\\&+\ddot S_{a\rho}v_a^\rho\dot v_{a\mu}+\frac{1}{3}\dot S_{a\rho}\ddot v_a^\rho v_{a\mu}\Big)\\&+\lambda^2/2(\dot S_{a\mu}-\dot S_{a\rho}v_a^\rho v_{a\mu})\Big\}\\&+g_a\lambda^2/2\Big\{\int_{-\infty}^{\tau}S_{a\mu}\frac{J_2(\lambda s)}{s^2}d\tau_a\\&-\int_{\tau}^{\infty}S_{a\mu}\frac{J_2(\lambda s)}{s^2}d\tau_a\Big\}\\&-g_a\frac{\lambda^3}{2}\Big\{\int_{-\infty}^{\tau}s_{a\mu}s_a^\nu S_{a\nu}\frac{J_3(\lambda s)}{s^3}d\tau_a\\&-\int_{\tau}^{\infty}s_{a\mu}s_a^\nu S_{a\nu}\frac{J_3(\lambda s)}{s^3}d\tau_a\Big\}.\end{aligned} \tag{19}$$

It is further observed that the fields defined by (16) and (17), satisfy the usual equations for the scalar meson field. Following Bhabha[5] the scattering of meson field by the particles can be easily calculated.

It is found that as a result of the additional terms in (13) and (19), the moment of inertia due to the field reactions does not appear in the scattering cross-sections. This is easily understood, because, in the theory of action at a distance, such field reaction terms are automatically excluded.

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1) J. A. Wheeler and R. P. Feynman, Rev. Mod. Phys. **17** (1945), 157; **21** (1949), 425.
2) H. Kanazawa, Prog. Theor. Phys. **5** (1950), 1050.
3) P. Havas, Phys. Rev. **87** (1952), 309.
4) R. C. Majumdar and S. Gupta, Phys. Rev. **75** (1949), 1788.
5) H. J. Bhabha, Proc. Roy. Soc. A. **178** (1941), 314.

On the Meson Wave Equation in de Sitter Space

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Recently S. A. Raje[1] has given an interesting discussion about the linear wave equation for mesons in de Sitter space, which approaches to Kemmer's equation for mesons in Minkowski space when the space becomes flat. In this note it is shown that this equation is essentially the same as the one proposed by us formerly[2] although without referring to physical quantities.

Wave equations for electrons and photons in de Sitter space were discussed by Dirac[3] for the first time. Wave equations for particles with arbitrary spin values, which approach to the wave equations of Bhabha[4] in Minkowski space when the space becomes flat, were introduced by us[2] using the five dimensional spinor analysis. In particular for mesons these equations approach then to Kemmer's equations, for the latter is a special case of Bhabha's equation for arbitrary spin values.

We proposed as general wave equation for arbitrary spin values

$$\{a^{\lambda\mu}m_{\lambda\mu}-2Rz\}\psi=0, \tag{1}$$

and put

$$a^{\lambda\mu}=I^{\lambda\mu}, \tag{2}$$

where $I^{\lambda\mu}$'s are the representarion matrices of infinitesimal transformations, concerning to x^{λ}-x^{μ} plane rotation, of the so-called de Sitter group. The condition for $I^{\lambda\mu}$ to be such ones is that the next commutation relation holds.

$$[I^{\lambda\mu}, I^{\rho\sigma}]=-g^{\lambda\rho}I^{\mu\sigma}+g^{\lambda\sigma}I^{\mu\rho}+g^{\mu\rho}I^{\lambda\sigma}-g^{\mu\sigma}I^{\lambda\rho}. \tag{3}$$

The wave function ψ is the irreducible spinor, in five dimensions[5], which transforms according to the representation generated by $I^{\lambda\mu}$. If we denote with $S^{\lambda\mu}(\theta)$ the transformation matrix of ψ concerning to the x^{λ}-x^{μ} plane rotation by angle θ, the next relations hold:

$$I^{\lambda\mu}=\left(\frac{\partial S^{\lambda\mu}(\theta)}{\partial\theta}\right)_{\theta=0}, \tag{4}$$

$$S^{\lambda\mu}(\theta)=e^{I^{\lambda\mu}\cdot\theta}. \tag{5}$$

When spinor transformation $S^{\lambda\mu}(\theta)$ is known, we can obtain $I^{\lambda\mu}$ by using (4). When a set of matrices $I^{\lambda\mu}$'s is known, we can obtain spinor transformation by using (5). For example fields of electrons, vector mesons and scalar mesons are those of the first rank spinors, the second rank symmetric spinors and the second rank antisymmetric spinors respectively, namely concerning to the irreducible representations $D\left(\frac{1}{2},\frac{1}{2}\right)$, $D(1,0)$ and $D(1,1)$ of the five dimensional rotational group. The spinor transformations in these cases are known by virtue of the five dimensional spinor calculus[5], so we can calculate $I^{\lambda\mu}$ and fix $a^{\lambda\mu}$ for these cases.

For spinor fields of electrons we have

$$I^{\lambda\mu}=\frac{1}{2}[a^{\lambda}, a^{\mu}], \tag{6}$$

$$a^{k}=\gamma^{k}\ (k=1,2,3,4),\quad a^{5}=\gamma^{1}\gamma^{2}\gamma^{3}\gamma^{4}, \tag{7}$$

$$a^{\lambda}a^{\mu}+a^{\mu}a^{\lambda}=2g^{\lambda\mu},\ (\lambda,\mu=1,2,3,4,5) \tag{8}$$

where γ^{k}'s are Dirac's matrices. Then the equation (1) becomes the electron field introduced by Dirac[3]. Indeed the transformation of the first rank spinor in

n dimensions are generated by (6) with α^λ satisfying (8), λ, μ running to n.

For second rank spinor fields of mesons we have

(vector meson case)

$$I^{12}=\frac{1}{2}\times$$

$$\begin{pmatrix} 0 & -\sqrt{2} & 0 & & & & & & & \\ \sqrt{2} & 0 & -\sqrt{2} & & & & & & & \\ 0 & \sqrt{2} & 0 & & & & & & & \\ & & & 0 & -\sqrt{2} & 0 & & & & \\ & & & \sqrt{2} & 0 & -\sqrt{2} & & & & \\ & & & 0 & \sqrt{2} & 0 & & & & \\ & & & & & & 0 & -1 & 1 & 0 \\ & & & & & & -1 & 0 & 0 & -1 \\ & & & & & & 1 & 0 & 0 & -1 \\ & & & & & & 0 & 1 & 1 & 0 \end{pmatrix},$$

$\cdots\cdots$, (9·a)

(scalar meson case)

$$I^{12}=\begin{pmatrix} 0 & -1 & -1 & 0 & \\ 1 & 0 & 0 & -1 & \\ 1 & 0 & 0 & -1 & \\ 0 & 1 & 1 & 0 & \\ & & & & 0 \end{pmatrix}, \cdots\cdots \quad (9\cdot b)$$

If we take these forms of $I^{\lambda\mu}$ as $\alpha^{\lambda\mu}$, we have wave equations of Bhabha's type, and wave functions are symmetric spinor

$$\psi=(\psi_{11}, \psi_{12}, \psi_{22}; \psi_{33}, \psi_{34}, \psi_{44}; \psi_{13}\psi_{14}\psi_{23}\psi_{24}) \quad (10\cdot a)$$

and antisymmetric spinor

$$\psi=(\psi_{13}, \psi_{14}, \psi_{23}, \psi_{24}; \psi_{12}+\psi_{34}), \quad (\psi_{12}-\psi_{34}=0) \quad (10\cdot b)$$

respectively.

In order to have wave equations of Kemmer's type we perform the following transformation

$$\phi_1=\frac{i}{\sqrt{2}}(\psi_{11}-\psi_{22}+\psi_{33}-\psi_{44}),$$

$$\phi_2=i(\psi_{12}+\psi_{34}),$$

$$\phi_3=\frac{1}{\sqrt{2}}(\psi_{11}+\psi_{22}+\psi_{33}+\psi_{44}),$$

$$\phi_4=\frac{1}{\sqrt{2}}(\psi_{11}-\psi_{22}-\psi_{33}+\psi_{44}),$$

$$\phi_5=\psi_{12}-\psi_{34},$$

$$\phi_6=\frac{i}{\sqrt{2}}(\psi_{11}+\psi_{22}-\psi_{33}-\psi_{44}),$$

$$\phi_7=-i(\psi_{13}-\psi_{24}),$$

$$\phi_8=i(\psi_{14}+\psi_{23}),$$

$$\phi_9=-(\psi_{13}+\psi_{24}),$$

$$\phi_{10}=-i(\psi_{14}-\psi_{23}), \quad (11\cdot a)$$

$$\phi_1'=\frac{-i}{\sqrt{2}}(\psi_{13}-\psi_{24}),$$

$$\phi_2'=\frac{i}{\sqrt{2}}(\psi_{14}+\psi_{23}),$$

$$\phi_3'=\frac{1}{\sqrt{2}}(\psi_{13}+\psi_{24}),$$

$$\phi_4'=\frac{i}{\sqrt{2}}(\psi_{14}-\psi_{23}),$$

$$\phi_5'=\psi_{12}+\psi_{34} \quad (11\cdot b)$$

respectively. Then taking imaginary x^4 and writing the transformed $I^{\lambda\mu}$ as $\beta^{\lambda\mu}$ and Kemmer's β matrices of 10 and 5 dimensions[6] as $\beta_{(10)}$, $\beta_{(5)}$, we have

$$\beta^{\chi 5}=\beta^{\chi}{}_{(10)} \quad (\chi=1, 2, 3, 4),$$

$$\beta^{12}=\begin{pmatrix} 0 & 1 & 0 & & & & & & & \\ -1 & 0 & 0 & & & & & & & \\ 0 & 0 & 0 & & & & & & & \\ & & & 0 & 1 & 0 & & & & \\ & & & -1 & 0 & 0 & & & & \\ & & & 0 & 0 & 0 & & & & \\ & & & & & & 0 & 1 & 0 & \\ & & & & & & -1 & 0 & 0 & \\ & & & & & & 0 & 0 & 0 & \\ & & & & & & & & & 0 \end{pmatrix},$$

$$\beta^{13}=\begin{pmatrix} 0 & 0 & 1 & & & & & & & \\ 0 & 0 & 0 & & & & & & & \\ -1 & 0 & 0 & & & & & & & \\ & & & 0 & 0 & 1 & & & & \\ & & & 0 & 0 & 0 & & & & \\ & & & -1 & 0 & 0 & & & & \\ & & & & & & 0 & 0 & 1 & \\ & & & & & & 0 & 0 & 0 & \\ & & & & & & -1 & 0 & 0 & \\ & & & & & & & & & 0 \end{pmatrix},$$

$$\beta^{23}=\begin{pmatrix}0&0&0&&&&&&&&&\\0&0&1&&&&&&&&&\\0&-1&0&&&&&&&&&\\&&&0&0&0&&&&&&\\&&&0&0&1&&&&&&\\&&&0&-1&0&&&&&&\\&&&&&&0&0&0&&&\\&&&&&&0&0&1&&&\\&&&&&&0&-1&0&&&\\&&&&&&&&&0&&\\&&&&&&&&&&0&\\&&&&&&&&&&&0\end{pmatrix},$$

$$\beta^{14}=\begin{pmatrix}&&&0&0&0&&&&&&\\&&&0&0&1&&&&&&\\&&&0&-1&0&&&&&&\\0&0&0&&&&&&&&&\\0&0&-1&&&&&&&&&\\0&1&0&&&&&&&&&\\&&&&&&&&&1&&\\&&&&&&&&&0&&\\&&&&&&&&&0&&\\&&&&&&1&0&0&0&&\\&&&&&&&&&&0&\\&&&&&&&&&&&0\end{pmatrix},$$

$$\beta^{24}=\begin{pmatrix}&&&0&0&-1&&&&&&\\&&&0&0&0&&&&&&\\&&&1&0&0&&&&&&\\0&0&1&&&&&&&&&\\0&0&0&&&&&&&&&\\-1&0&0&&&&&&&&&\\&&&&&&&&&0&&\\&&&&&&&&&1&&\\&&&&&&&&&0&&\\&&&&&&0&1&0&0&&\\&&&&&&&&&&0&\\&&&&&&&&&&&0\end{pmatrix},$$

$$\beta^{34}=\begin{pmatrix}&&&0&1&0&&&&&&\\&&&-1&0&0&&&&&&\\&&&0&0&0&&&&&&\\0&-1&0&&&&&&&&&\\1&0&0&&&&&&&&&\\0&0&0&&&&&&&&&\\&&&&&&&&&0&&\\&&&&&&&&&0&&\\&&&&&&&&&1&&\\&&&&&&0&0&1&0&&\\&&&&&&&&&&0&\\&&&&&&&&&&&0\end{pmatrix},\qquad(12\cdot a)$$

(unwritten rectangulars are filled with zero)

and

$$\beta^{\varkappa 5}=\beta^{\varkappa}{}_{(5)}\qquad(\varkappa=1,\ 2,\ 3,\ 4),$$

$$\beta^{12}=\begin{pmatrix}0&1&0&0&&\\-1&0&0&0&&\\0&0&0&0&&\\0&0&0&0&&\\&&&&0&\\&&&&&0\end{pmatrix},\quad\beta^{14}=\begin{pmatrix}0&0&0&1&&\\0&0&0&0&&\\0&0&0&0&&\\1&0&0&0&&\\&&&&0&\\&&&&&0\end{pmatrix},$$

$$\beta^{13}=\begin{pmatrix}0&0&1&0&&\\0&0&0&0&&\\-1&0&0&0&&\\0&0&0&0&&\\&&&&0&\\&&&&&0\end{pmatrix},\quad\beta^{24}=\begin{pmatrix}0&0&0&0&&\\0&0&0&1&&\\0&0&0&0&&\\0&1&0&0&&\\&&&&0&\\&&&&&0\end{pmatrix},$$

$$\beta^{23}=\begin{pmatrix}0&0&0&0&&\\0&0&1&0&&\\0&-1&0&0&&\\0&0&0&0&&\\&&&&0&\\&&&&&0\end{pmatrix},\quad\beta^{34}=\begin{pmatrix}0&0&0&0&&\\0&0&0&0&&\\0&0&0&1&&\\0&0&1&0&&\\&&&&0&\\&&&&&0\end{pmatrix},$$

(12·b)

respectively. Taking these $\beta^{\lambda\mu}$ as $a^{\lambda\mu}$ of (1), we have the equation of Kemmer's type.

In order to have equations of Yukawa's type, we have only to put

$$\begin{pmatrix}0&F_{12}&F_{13}&F_{14}&F_{15}\\&0&F_{23}&F_{24}&F_{25}\\&&0&F_{34}&F_{35}\\&&&0&F_{45}\\&&&&0\end{pmatrix}=\begin{pmatrix}0&-\phi_6&\phi_5&\phi_1&-i\phi_7\\&0&-\phi_4&\phi_2&-i\phi_8\\&&0&\phi_3&-i\phi_9\\&&&0&-i\phi_{10}\\&&&&0\end{pmatrix},\qquad(13\cdot a)$$

and

$$(U_1,\ U_2,\ U_3,\ U_4,\ U_5)=(\phi_1',\ \phi_2',\ \phi_3',\ \phi_4',\ -i\phi_5')\qquad(13\cdot b)$$

respectively, and we obtain the equation reported formerly.

$$m_\lambda{}^\mu F_{\mu\nu}-m_\nu{}^\mu F_{\mu\lambda}=R\varkappa F_{\lambda\nu},\qquad(14\cdot a)$$

$$m_\mu{}^\nu U_\nu=R\varkappa U_\mu.\qquad(14\cdot b)$$

In the previous paper we reported only this last form of Yukawa's type omitting these calculations and above all the second form of Kemmer's type.

Now the meson wave equation proposed by S. A. Raje is

$$\{S^{\lambda\mu}m_{\lambda\mu}-2R\varkappa\}\psi=0,\qquad(15)$$

$$S^{\mu\nu}=\beta^\mu\beta^\nu-\beta^\nu\beta^\mu,\qquad(16)$$

$$\beta^\mu\beta^\nu\beta^\lambda+\beta^\lambda\beta^\nu\beta^\mu=g^{\mu\nu}\beta^\lambda+g^{\lambda\nu}\beta^\mu.\qquad(17)$$

We can easily show that this is included in our equation (1), because $S^{\lambda\mu}$ of (16) with β^μ's satisfying (17) can be shown to satisfy the commutation relation (3). Thus $S^{\lambda\mu}$ is a special representation of $I^{\lambda\mu}$, and we can say that the irreducible representations give the matrices $\beta^{\lambda\mu}$ of (12·a) or (12·b) as the form of $S^{\lambda\mu}=\beta^\lambda\beta^\mu-\beta^\mu\beta^\lambda$, if the note gives a concrete form to the physical quantities introduced by Raje such as the current vector and the energy momentum tensor, for they are written with $S^{\lambda\mu}$ composed from β^μ's and $S^{\lambda\mu}$'s are realized by the matrices $\beta^{\lambda\mu}$'s of (12·a), (12·b), even if β^μ itself is not so.

We have recently introduced the wave equation for arbitrary spins which approaches to Dirac-Fierz's equation in Minkowski space when the space becomes flat, using the further developed calculus of five dimensional spinor. Some solutions of wave equations, in particular static solutions such as Coulomb and Yukawa potentials in small regions, are also obtained. This will appear in this journal shortly.

1) Raje, Prog. Theor. Phys. **8** (1952), 384.
2) Goto, Prog. Theor. Phys. **6** (1951), 1013.

In this paper equations (12) and (15) were miswritten and they must be corrected by replacing with (13·a) and (13·b) in the present report respectively.

3) Dirac, Ann. Math. **36** (1935), 657.
4) Bhabha, Rev. Mod. Phys. **17** (1945), 200.
5) Goto, Prog. Theor. Phys. **5** (1950), 43.
6) Kemmer, Proc. Roy. Soc. **A. 173** (1939), 92.

On the Interactions of the Second Kind

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As is well-known, for interactions of the first kind the renormalization procedure with the use of usual perturbation method succeeds to give the consistent non-singular theory[1], but for those of the second kind it can not give the closed form. On the other hand the recent experimental facts seem to suggest the existence of interactions of the latter kind and so it becomes the important problem how to treat the divergences arising from them.

If we have the theory in which the unitarity of the S-matrix is guaranteed, the strong singularities appearing in the lower order perturbation calculations may altogether be compensated by the strong damping effect coming from the higher order terms. Such a consideration was just the starting-point of Heitler and Wilson[2] in their theory of radiation damping. Since the field reaction due to the interaction of the second kind gives the large damping effect we can expect that the non-singular theory may be obtained by appropriately taking into account the large field reaction due to the interaction of this kind. In this note we show that such an expectation is actually the case when we use the suitable interactions of the second kind as the field corrections. The secondary introduction of them may be regarded as a formal extension of the usual method of renormalization theory (counter terms) or rather a generalization of the idea of the mixed-field theory (auxiliary fields).

In general, we can take into account some parts of the field reaction by using the corrected propagation function[3] $\Delta^{\alpha}{}_{F}{}'$ of α-field, which is given by

$$\Delta^{\alpha\prime}_{F}(k)=\Delta^{\alpha}_{F}(k)/(1-\Delta^{\alpha}_{F}(k)\textstyle\sum_{c}^{\alpha}(k)), \quad (1)$$

where $\sum_{c}{}^{\alpha}(k)$ is the finite remainder of the m^{α}-th order proper self-energy part $\sum^{\alpha}(k)$ of α-field (: attached momentum) due to an interaction $H_{l_{\alpha}}$[4]. Since $\sum^{\alpha}$ usually contains divergent terms, we must cancel them by using the appropriate counter terms, the number of which is, of course, finite for a given value of $m^{\alpha}\eta_{l_{\alpha}}$. When the coupling constant of $H_{l_{\alpha}}$ is of the dimension of (length)$^{\delta}$, $\Delta^{\alpha}{}_{F}{}'(k)$, for large k, behaves like

$$\Delta^{\alpha\prime}_{F}(k)\sim\begin{cases}k^{b^{\alpha}-2} & \text{for } \eta_{l_{\alpha}}\leqq 0,\\ k^{b^{\alpha}-2-m^{\alpha}/l_{\alpha}} & \text{for } \eta_{l_{\alpha}}>0.\end{cases} \quad (2)$$

As has been expected, the damping factor $k^{-m^{\alpha}\eta_{l_{\alpha}}}$ appears only when we adopt the interaction of second kind for the correction of $\Delta^{\alpha}{}_{F}$.

Next, we shall consider a system of fields coupled by a set of interactions $H=\sum_{l}H_{l}$, some of which are supposed to belong to the second kind, and correct the propagation function of the α-field to the m^{α}-th order with respect to the interaction $H_{l_{\alpha}}$. Then, we can prove the following fact: When the S-matrix elements are calculated exclusively in terms of the corrected propagation functions $\Delta^{\alpha}{}_{F}{}'$ any ultra-violet divergences do not appear in these calculations provided that the following conditions are satisfied for all the interactions;

$$\frac{1}{2}m^{\alpha}\eta_{l_{\alpha}}-e^{\alpha}>\frac{1}{2}\{\eta_{l}-\sum_{\beta}\lambda_{l}^{\beta}e^{\beta}\}+2, \quad (3)$$

where $e^{\alpha}\equiv d^{\alpha}+\frac{1}{2}b^{\alpha}+1$ and d^{α} is the minimum degree of the derivation operator operating on U^{α} in H. Thus, (3) is a sufficient condition for the closure of the theory. It is easily shown that the condition (3) is actually satisfied when we suitably choose the

interaction H_{l_α} and m^α. For $m^\alpha=1$, the special consideration becomes necessary from the requirement of gauge invariance of the theory. In this case (3) is to be replaced by a somewhat weaker condition and then the theory contains a finite number of primitive divergences.

The limited number of divergences can be removed by the method familiar in the usual renormalization theory and we are led to the closed non-singular theory.

According to the type of interactions H_{l_α} used for the correction we shall classify our method into the following three cases:

(A) H_{l_α}'s are ordinary interactions having the field quantities more than 3. $(m^\alpha \geqq 2)$,

(B_1) H_{l_α}'s are two-vertex interactions such as $fF(\partial)U^\alpha U^\alpha$ $(m^\alpha=1)$.

(B_2) H_{k_α}'s are two-vertex interactions such as $fF(\partial)U^\alpha U^\beta$ $(\alpha \neq \beta)$ $(m^\alpha=2)$.

In the case (A), $\sum^\alpha$ contains, in general, the diverging part $\sum^\alpha{}_\infty$, which is to be subtracted when $\sum^\alpha{}_c$ is substituted into (1). When H_{l_α}'s are three-vertex interactions, such subtractions are easily performed by the 2-vertex counter terms. In cases (B_1) and (B_2) $\sum^\alpha$ does not diverge. Hence, the subtraction is unnecessary and, if the conditions (3) are satisfied, we can obtain the completely convergent theories.

Using our method, we can obtain, for instance, the completely convergent quantum electrodynamics and non-singular ps (pv) meson theory. Furthermore, the very success of Fermi theory of β-disintegration can be easily understood from our view-point.

Finally, we shall notice some of the characteristic features of our method. Since the propagation function (1) has usually new poles, we are led to the results similar to the resonance effects[5]. In the case (B_1), if we regard $fF(\partial)U^\alpha U^\alpha$ as a part of the free Lagrangian of the corresponding field (i.e. non-local action[6]), we can obtain from the outset the same propagation function as (1). It should be noticed, however, that the quantum field theory in which $fF(\partial)U^\alpha U^\alpha$ is treated as the interaction term is based on the different quantization method from that of the theory of non-local action and so the real production of negative energy particles does not occur at all[7]. There occur similar circumstances in the case (B_2), too, for we can diagonalize the free Lagrangian, including the term $fF(\partial)U^\alpha U^\beta$, with respect to a set of suffices α and β. The use of the corrected propagation function $\Delta^\alpha{}_{F'}$ corresponds to the theory using the corrected field quantity $U^{\alpha\prime}$, for which there holds $\langle P(U^{\alpha\prime}(x), U^{\alpha\prime}(x'))\rangle_0 = \Delta^\alpha{}_{F'}(x-x')$. But, we have not yet found the consistent formulation of our method, which has no recourse to the Feynman diagrams. The detailed account will appear in this journal.

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1) We call a theory "closed" or "completely convergent" according as all divergences thereof can be removed by the finite number of counter interactions or any divergence does not appear at all. Further, we call these two cases "non-singular" theories.
2) W. Heitler, Proc. Camb. Phil. Soc. **37** (1941), 291; A. H. Wilson, ibid. **37** (1941), 301.
3) In order to take into account the field reactions there may be various possible ways, but we adopt, in this note, the method of the corrected propagation functions, for it is the most simple one. See further N. Hu, Phys. Rev. **80** (1950), 1109.
4) In this note the same notations shall be used as in our previous paper: S. Sakata, H. Umezawa and S. Kamefuchi, Prog. Theor. Phys. **7** (1952), 377.
5) As to the definition of $\Delta^\alpha{}_{F'}$, which is given as the solution of the integral equation $\Delta^\alpha{}_{F'} = \Delta^\alpha{}_F + \Delta^\alpha{}_F \sum_c{}^\alpha \Delta^\alpha{}_{F'}$, there appear some ambiguities in connection with the zero-point of $(1-\Delta^\alpha{}_F \sum_c{}^\alpha)$. We shall discuss this point in detail in the forthcoming paper.
6) A. Pais and G. E. Uhlenbeck, Phys. Rev. **79** (1950), 145.
7) Y. Takahashi and H Umezawa, unpublished results.

On the π-P Scattering

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Recent experiments on π nucleon scattering show that $\sigma(\pi^+)$ is considerably bigger than the $\sigma(\pi^-)$. It is difficult to understand this situation from weak coupling theory. Brueckner has calculated the ratio

on the basis of strong coupling theory with the assumption that the scattering is only due to a state with an isotopic spin $I=3/2$, and obtained the result

$$\sigma(\pi^+) : \sigma(\pi^-) = 9 : 1,$$

which is rather in good agreement with the experiment.

But it seems more reasonable to understand the situation as a result of the interference between $I=3/2$ state and $I=1/2$ state.

$I=3/2$ states (A) and $I=1/2$ states (B) are given in the next table.

$I=3/2$	$I=1/2$
$A^{++}=P\pi^+$	
$A_+=\left(\sqrt{\frac{2}{3}}P\pi^0 + \sqrt{\frac{1}{3}}N\pi^+\right)$	$B^+=\left(\sqrt{\frac{1}{3}}P\pi^0 - \sqrt{\frac{2}{3}}N\pi^+\right)$
$A^0=\left(\sqrt{\frac{1}{3}}P\pi^- + \sqrt{\frac{2}{3}}N\pi^0\right)$	$B^0=\left(\sqrt{\frac{2}{3}}P\pi^- - \sqrt{\frac{1}{3}}N\pi^0\right)$
$A^-=N\pi^-$	

From this table

$$P\pi^+ = A^{++},$$

$$P\pi^- = \sqrt{\frac{1}{3}}A^0 + \sqrt{\frac{2}{3}}B^0.$$

Using those wave functions, scattering S-matrices are calculated.

$$S(\pi^+) = S_{3/2},$$

$$S(\pi^-) = \frac{1}{3}S_{3/2} + \frac{2}{3}S_{1/2},$$

where

$$S_{3/2} = (A|S|A),$$

$$S_{1/2} = (B|S|B).$$

It is reasonable to suppose that $S_{3/2}$ and $S_{1/2}$ are of equal order and with opposite sign. Then

$$S(\pi^+) : S(\pi^-) = 3 : 1,$$

$$\sigma(\pi^+) : \sigma(\pi^-) = 9 : 1.$$

Errata

The figure in page 576 (Vol. 8, No. 5) should be inserted in the article "π-D Scattering and Strong Coupling Theory" (P. 573) by H. Miyazawa and S. Matsuyama.

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